#### => d his

(FILE 'HOME' ENTERED AT 09:59:03 ON 27 DEC 2007)

FILE 'REGISTRY' ENTERED AT 10:00:33 ON 27 DEC 2007

L1 STRUCTURE UPLOADED

L2 12 S L1

L3 282 S L1 FUL

FILE 'CAPLUS' ENTERED AT 10:01:14 ON 27 DEC 2007

L4 146 S L3

FILE 'REGISTRY' ENTERED AT 10:03:52 ON 27 DEC 2007

L5 STRUCTURE UPLOADED

L6 19 S L5

L7 STRUCTURE UPLOADED

L8 19 S L7

L9 66913 S CAN

FILE 'REGISTRY' ENTERED AT 11:05:04 ON 27 DEC 2007

L10 19 S L7

L11 261 S L7 FUL

L12 6 SEARCH L7 CSS SUB=L11 FUL

FILE 'CAPLUS' ENTERED AT 11:07:27 ON 27 DEC 2007

L13 3 S L12

## => d bib abs hitstr 1-3

L13 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1986:148472 CAPLUS

DN 104:148472

TI Synthesis of amine derivatives

IN Masuko, Fujio; Katsura, Tadashi

PA Sumitomo Chemical Co., Ltd., Japan

SO U.S., 13 pp. Cont.-in-part of U.S. Ser. No. 65,429, abandoned.

CODEN: USXXAM DT Patent

LA English

FAN. CNT 2

ran.	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
			<del></del>		
ΡI	US 4536599	Α	19850820	US 1979-90479	19791101
	JP 55028959	Α	19800229	JP 1978-102614	19780822
	JP 61055488	В	19861128		
	JP 55033442	Α	19800308	JP 1978-106541	19780830
	JP 62000905	В	19870110		
PRAI	JP 1978-102614	Α	19780822		
	JP 1978-106541	Α	19780830		
	US 1979-65429	A2	19790810		
OS	MARPAT 104:148472		•		
GI					

$$R^{1}$$
 (CHR3)  $n$ CHR  $R^{2}$ 

chain nodes:

2 3 15 16 17 19 20 21 22 23 24 25 29 31 ring nodes:

1 4 5 6 7 8 9 10 11 12 13 14

chain bonds:

1-2 2-3 2-19 3-4 3-15 15-16 15-17 20-21 20-22 23-24 24-25 ring bonds :

1-5 1-9 4-10 4-14 5-6 6-7 7-8 8-9 10-11 11-12 12-13 13-14

3:3 E exact RC ring/chain

# Match level:

1:Atom 2:CLASS3:CLASS4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:/ 13:Atom 14:Atom 15:CLASS16:CLASS17:CLASS19:CLASS20:CLASS2 24:CLASS25:CLASS29:CLASS30:Atom 31:CLASS32:Atom

Diphenylalkylamines I (R = NH2; R1-R5 = H, halo, OH, trihalomethyl, Ph, PhO, PhS, alkyl, alkenyl, alkoxy, alkylthio, dialkylamino, alkylsulfonyl; n = 2, 3), useful as pharmaceutical intermediates and optical resolution agents, were prepared by condensing R4R5C6H3CH2CN with R1R2C6H3(CHR3)nX (X = halo) in the presence of a base, hydrolysis of the resultant I (R = cyano) by H2O2 and a base in the presence of an organic quaternary ammonium salt, and Hofmann rearrangement of the resultant I (R = CONH2) in the presence of a base. Thus, 4-C1C6H4CH2CN, PhCH2Cl, Bu4NBr, and 25% aqueous NaOH reacted in PhMe to give 95% PhCH2CHRC6H4Cl-4 (II; R = cyano), which was hydrolyzed by aqueous NaOH-H2O2 in MeOH in the presence of Bu4NBr to give 98% II (R = CONH2). Rearrangement of the amide by Br-NaOH in MeOH gave 97% II (R = NH2) (III), which was resolved by L-(+)-tartaric acid to give 50% resolution yield of 1-III.

IT 74533-40-7P 74533-41-8P 74533-42-9P

74533-47-4P 74533-54-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction with hypohalite)

RN 74533-40-7 CAPLUS

CN Benzenepropanamide, 4-methyl- $\alpha$ -(4-methylphenyl)- (CA INDEX NAME)

RN 74533-41-8 CAPLUS

CN Benzenepropanamide,  $\alpha$ -(4-chlorophenyl)-4-methyl- (CA INDEX NAME)

RN 74533-42-9 CAPLUS

CN Benzenepropanamide, α-(3-bromophenyl)-4-methyl- (CA INDEX NAME)

RN 74533-47-4 CAPLUS

CN Benzenepropanamide,  $\alpha$ -(3-hydroxyphenyl)-4-propyl- (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ &$$

RN 74533-54-3 CAPLUS

CN Benzenepropanamide, 2-ethyl- $\alpha$ -(3-methylphenyl)- (CA INDEX NAME)

L13 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1983:575329 CAPLUS

DN 99:175329

OREF 99:26889a,26892a

TI Oxidative decyanation of benzyl and benzhydryl cyanides. A simplified procedure

AU Kulp, Stuart S.; McGee, Michael J.

CS Dep. Chem., Moravian Coll., Bethlehem, PA, 18018, USA

SO Journal of Organic Chemistry (1983), 48(22), 4097-8

CODEN: JOCEAH; ISSN: 0022-3263

DT Journal

LA English

OS CASREACT 99:175329

AB The reaction of 24 examples of mono and disubstituted nitriles with atmospheric oxygen in Me2SO and either K2CO3 or lithium isopropylcyclohexylamide base at ambient temperature is reported. In 13 cases the oxidative decyanation product (ketone) was obtained in >90% yield. Thus, 1.00 g PhCH2CN was treated with 1.00 g K2CO3 in 30 mL Me2SO at room temperature to give 0.809 Ph2CO

(95% yield). Reaction half-lifes were determined for several nitriles.

IT 87184-36-9P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of, by oxidative decyanation of nitrile)

RN 87184-36-9 CAPLUS

CN Benzenepropanamide,  $\alpha$ -(4-chlorophenyl)-4-methoxy- (CA INDEX NAME)

L13 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1980:495018 CAPLUS

DN 93:95018

OREF 93:15221a,15224a

TI Synthesis of amides and amines

IN Masuko, Fujio; Katsura, Tadashi

PA Sumitomo Chemical Co., Ltd., Japan

SO Eur. Pat. Appl., 49 pp.

CODEN: EPXXDW

DT Patent

LA English

FAN. CNT 2

PAN.	PATENT NO.	KIND DATE	APPLICATION NO.	DATE
PI	EP 8532	A1 19800305	EP 1979-301696	19790820
	EP 8532 R: BE, CH, DE,	B1 19830720 , FR, GB, IT, NL, S	SE	•
	JP 55028959	A 19800229	JP 1978-102614	19780822
	JP 61055488 JP 55033442	B 19861128 A 19800308	JP 1978-106541	19780830
	JP 62000905	B 19870110	01 1976 100941	13700030
	EP 40896	A2 19811202	EP 1981-200767	19790820
	EP 40896	A3 19820203		
	EP 40896	B1 19840425 , FR, GB, IT, NL, S	2 F	
PRAI	JP 1978-102614	A 19780822	JE	
	JP 1978-106541	A 19780830		
	EP 1979-301696	A 19790820	,	
GI				

AB Amides I (R1, R2, R3, R4 = H, halo, OH, trihalomethyl, Ph, PhO, PhS, C1-6 alkyl, hydroxyalkyl, alkenyl, alkoxy, alkylthio, dialkylamino, alkylsulfonyl; R1R2 or R3R4 = ring; R3 = H or R1) were prepared by hydrolysis of the corresponding nitriles in presence of quaternary ammonium compds. and in aqueous alkaline H2O2. The amides I were converted to

corresponding amines by treatment with hypohalites. Thus, PhCH2CN with 4-MeC6H4CH4Cl gave PhCH(CN)CH2C6H4Me-4, which on hydrolysis in aqueous NaOH containing H2O2 and Bu4NOH gave PhCH(CONH2)CH2C6H4Me-4 (II). II in MeOH containing NaOH was treated with Br at 0° and a catalytic amount of Bu4NOH and the mixture refluxed to give PhCH2CH(NH2)CH2C6H4-Me.

IT 74533-40-7P 74533-41-8P 74533-42-9P

74533-47-4P 74533-54-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction with hypohalite)

RN 74533-40-7 CAPLUS

the

CN Benzenepropanamide, 4-methyl $-\alpha$ -(4-methylphenyl)- (CA INDEX NAME)

$$\begin{array}{c|c} \text{O} \\ \text{C-NH}_2 \\ \text{CH-CH}_2 \\ \text{Me} \end{array}$$

RN 74533-41-8 CAPLUS

CN Benzenepropanamide,  $\alpha$ -(4-chlorophenyl)-4-methyl- (CA INDEX NAME)

$$\begin{array}{c} \text{O} \\ \parallel \\ \text{C-NH}_2 \\ -\text{CH-CH}_2 \\ \end{array}$$

RN 74533-42-9 CAPLUS

CN Benzenepropanamide,  $\alpha$ -(3-bromophenyl)-4-methyl- (CA INDEX NAME)

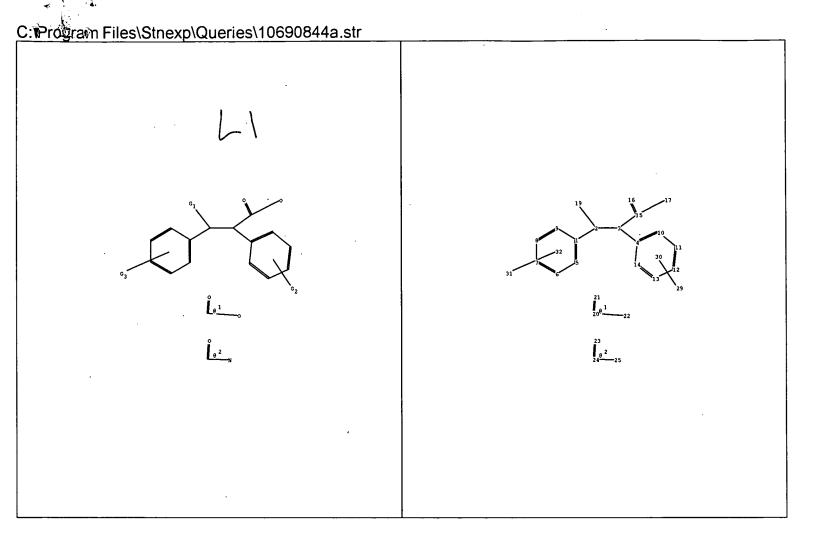
RN 74533-47-4 CAPLUS

CN Benzenepropanamide,  $\alpha$ -(3-hydroxyphenyl)-4-propyl- (CA INDEX NAME)

$$\begin{array}{c|c} & \circ & \\ & \parallel & \\ & \text{C-NH}_2 \\ & \text{CH-CH}_2 \\ & & \\$$

RN 74533-54-3 CAPLUS

CN Benzenepropanamide, 2-ethyl- $\alpha$ -(3-methylphenyl)- (CA INDEX NAME)



chain nodes:

2 3 15 16 17 19 20 21 22 23 24 25 29 31

ring nodes:

1 4 5 6 7 8 9 10 11 12 13 14

chain bonds:

1-2 2-3 2-19 3-4 3-15 15-16 15-17 20-21 20-22 23-24 24-25

ring bonds:

1-5 1-9 4-10 4-14 5-6 6-7 7-8 8-9 10-11 11-12 12-13 13-14

exact/norm bonds:

2-19 15-16 15-17 20-21 20-22 23-24 24-25

exact bonds:

1-2 2-3 3-4 3-15

normalized bonds:

1-5 1-9 4-10 4-14 5-6 6-7 7-8 8-9 10-11 11-12 12-13 13-14

G1:H,Ak,OH

G2:Ak,OH,SO2,NH,X,[\*1],[\*2]

G3:X,Ak,MeO,EtO,n-PrO,i-PrO,n-BuO,i-BuO,s-BuO,t-BuO,SO2,NH,[\*1],[\*2]

Connectivity:

₹3:3-E exact RC ring/chain

Match level:

1:Atom 2:CLASS3:CLASS4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:CLASS16:CLASS17:CLASS19:CLASS20:CLASS21:CLASS22:CLASS23:CLASS 24:CLASS25:CLASS29:CLASS30:Atom 31:CLASS32:Atom

=> d his

(FILE 'HOME' ENTERED AT 09:59:03 ON 27 DEC 2007)

FILE 'REGISTRY' ENTERED AT 10:00:33 ON 27 DEC 2007

L1 STRUCTURE UPLOADED

L2 12 S L1

L3 282 S L1 FUL

FILE 'CAPLUS' ENTERED AT 10:01:14 ON 27 DEC 2007

L4 146 S L3

=> d 11

L1 HAS NO ANSWERS

L1 STR

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \* Structure attributes must be viewed using STN Express query preparation.

 $\Rightarrow$  d bib abs hitstr 55-146

ANSWER 55 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1996:193712 CAPLUS 24:316690

L4 AN DN TI Synthesis of 1,3,6,8-tetramethoxy-cis-4b,5,9b,10-tetrahydroindeno[2,1-

Synthesis of 1, 5,8-terramethoxy-cis-46,3,96,10-tetranyoroindeno[2,1-a]indene-5,10-dione
Bianchi, D. E.: Alesso, E. N.: Iglesias, G. Y. Moltrasio
Departamento Quimica Organica, Universidad Buenos Aires Junin 956 (1113),
Buenos Aires, Argent.
Organic Preparations and Procedures International (1996), 28(2), 230-4
CODEN: OPPIAK: ISSN: 0030-4948
Organic Preparations and Procedures, Inc.
Journal

so

English CASREACT 124:316690

The title compound I was prepared in 5 steps from (3,5-dimethoxypheny)]acetonitrile. I will be used in an investigation of the synthesis of pallidol.
176386-39-39 176386-40-6p
RL: RCT (Reactant): 5FN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of tetramethoxyindenoindenedione)
176386-39-3 CAPLUS
Butanedioic acid, 2,3-bis(4-hydroxyphenyl)-, diethyl ester, (R\*,R\*)- (9CI)
(CA INDEX NAME)

Relative stereochemistry.

Itanedioic acid, 2,3-bis(4-hydroxyphenyl)-, diethyl ester, (R\*,S\*)- (9CI) (CA INDEX NAME)

ANSWER 56 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1995;402285 CAPLUS 122:290768
Some reactions of (3,4,5-trimethoxybenzylidene)-4-methoxyacetophenone Mahnoud, M. R.; Ebrahlm, Avatef E. F.; Abd-El-Hallm, M. S.; Radwan, A. M. Faculty Science, Ain Shams University, Cairo, Egypt Indian Journal of Heterocyclic Chemistry (1994), 4(2), 131-6 CODEN: IJCHEI; ISSN: 0971-1627 Journal English Some new pyrazolines have been prepared by the reaction of (3,4,5-trimethoxybenzylidene)-4-methoxyacetophenone (1) with hydrazines in different media. Unexpected bromination is observed on treatment of 1 with bromine to give the pentabromo derivative, which was reacted with hydrazine hydrate and hydroxylamine hydrochloride. The behavior of 1 towards Et phenylacetate, Et cyanoacetate, and di-Et homophthalate under Michael conditions has also been studied. Reaction of 1 with thioglycollic and thiobarbituric acids have also been studied. 163074-81-5P RL: SPN (Synthetic preparation); PREP (Preparation) (reactions of (trimethoxybenzylidene)methoxyacetophenone) 163074-81-5 CAPLUS Benzenepentanoic acid, a-[2-(ethoxycarbonyl)phenyl]-4-methoxy-6-oxo-β-(3,4,5-trimethoxyphenyl)-, ethyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 55 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN Relative stereochemistry. (Continued)

ANSWER 57 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1995;363883 CAPLUS 122:329535 Differentiation of meso- and dl-α-polysubstituted dibenzyl compounds

L4 AN DN TI

so

122:329335

Differentiation of meso- and dl-α-polysubstituted dibenzyl compounds by IR spectroscopy

Zhang, Bin: Jia, Zhishing; Qi, Chenze
Department of Chemistry, Lanzhou University, Lanzhou, 730000, Peop. Rep.
China
Lanzhou Daxue Xuebao, Ziran Kexueban (1994), 30(1), 68-71
CODEN: LCTHAF: ISSN: 0455-2059
Lanzhou Daxue
Journal
Chinese
Meso- and dl-diethyl-2,3-dicyano-2,3-di(p-X substituted phenyl) succinates
(X = OMe, CHJ, H, Cl, NO2) were studied by IR spectroscopy. The vibration
vavenumbers of meso-isomers are higher at vc=o and lower at vc-o-c
than those of the corresponding dl-isomers.
139257-67-3 139257-68-4 139257-70-8,
meso-Diethyl-2,3-dicyano-2,3-di(p-chlorophenyl) succinate
139257-17-19
RL: ANT (Analyte) PRP (Properties): ANST (Analytical study)
(differentiation of meso- and dl-α-polysubstituted dibenzyl
compds. by IR spectroscopy)
139257-67-3 CAPLUS
Butanedioic acid, 2,3-dicyano-2,3-bis(4-methylphenyl)-, diethyl ester,
(2R,3S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

Relative stereochemistry.

139257-68-4 CAPLUS Butanedioic acid, 2,3-dicyano-2,3-bis(4-methylphenyl)-, diethyl ester, (ZR,JR)-rel- (9CI) (CA INDEX NAME)

139257-70-8 CAPLUS Butanedioic acid, 2,3-bis(4-chlorophenyl)-2,3-dicyano-, diethyl ester, (ZR,35)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

ANSWER 57 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN

139257-71-9 CAPLUS Butanedioic acid, 2,3-bis(4-chlorophenyl)-2,3-dicyano-, diethyl ester, (ZR, JR)-rel- (9C1) (CA INDEX NAME)

Relative stereochemistry.

ANSWER 58 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN

ANSWER 58 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1994:680346 CAPLUS 121:280346

L4 AN DN TI

121:280346
Mass spectra of dL-diethyl 2,3-dicyano-2,3-bis(p-substituted phenyl) succinates
Li, Haiquan; Qi, Chenze; Zai, Jianjun; Zhao, Fanzhi; Chen, Nenyu; Hao, Xiumei; Yang, Dilun
Dep. Chem., Lanzhou Univ., Lanzhou, 730000, Peop. Rep. China
Lanzhou Daxue Xuebao, Ziran Kexueban (1993), 29(3), 142-4
CODEN: LCTHAF; ISSN: 0455-2059
Journal ΑU

CS SO

DT LA GI

The mass spectral of title compds. I (X = H, Cl, Me, MeO, NO2) were studied by means of low resolution EIMS and high resolution accuracy mass measuring MS. The fragmentation mechanism of the di-Et esters and structures of characteristic ions formed were discussed.

139257-68-4 139257-71-9

RL: PRP (Properties)
(mass spectra of di-Et dicyano(diphenyl) succinates)
139257-68-4 CAPLUS

Butanedioic acid. 2,3-dicyano-2,3-bis(4-methylphenyl)-, diethyl ester, (2R,3R)-rel- (9C1) (CA INDEX NAME)

Relative stereochemistry.

139257-71-9 CAPLUS Butanedioic acid, 2,3-bis(4-chlorophenyl)-2,3-dicyano-, diethyl ester, (ZR,3R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

ANSVER 59 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1994:500056 CAPLUS 121:100056 Bivalent Ligands as probes of estrogen receptor action Bivalent Ligands as probes of estrogen receptor action Bergmann, Kathryn E.; Wooge, Cynthia H.; Carlson, Kathryn E.; Katzenellenbogen, Benita S.; Katzenellenbogen, John A. Dep. Chem., Univ. Illinois, Urbana, IL, 61801, USA Journal of Steroid Biochemistry and Molecular Biology (1994), 49(2-3), 139-52 CODEN: JSBBEZ; ISSN: 0960-0760 Journal English

Journal English

The estrogen receptor (ER) is a hormone-regulated transcription factor which is thought to bind to specific DNA sequences as a homodimer. To better understand structural requirements for dimerization and its functional role in ER action, the authors synthesized a series of bivalent ligands based on the non-steroidal estrogen hexestrol (I). These mol. probes join two hexestrol mols. of the erythro (E. active) configuration with either 4 or 8 carbon linkers (II) (designated E-4-E (X = (CH2)4) and E-8-E (X = (CH2)8) series, resp.], or with longer linkers comprised of ethylene glycol units II (E-eg-E (X = CH2(CH2OCH2)nCH2, n = 1-4) series). Several other bir and sonovalent control compds. were prepared The bivalent ligands bind to ER with a relative affinity 1-78 that the estradiol. While most of the ligands demonstrated normal monophasic displacement curves in competitive binding assays with [3H] estradiol, uncharacteristic biphasic competitive binding curves were seen for some of the ligands, indicating possible structure-specific, neg. site-site interaction. In ER-deficient Chinese hamster ovary (CHO) cells transfected with an expression vector encoding ER, one series of bivalent ligands (E-4-E) had little stimulatory activity and inhibited transcription stimulated by hexestrol, as determined by a transient transfection assay using an estrogen-responsive reporter gene construct ((ERE)-TATA-CAT, containing two estrogen response elements linked to a TATA promoter and the chloramphenicol acetyl transferase reporter gene). Monovalent or control bivalent ligands failed to antagonize hexestrol-stimulated activity and were as fully active as hexestrol itself. Studies performed in MCP-7 human breast cancer cells, which contain endogenous ER, yielded similar bioactivity profiles for the E-4-E bivalent inhibitory ligands, showing then to be effective estrogen antagonists, when using either induction of

ANSWER 59 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) progesterone receptor or (ERE)2-TATA-CAT transcriptional activation as the endpoint. The E-8-E ligand, however, acted as partial agonist/antagonist of ERE-reporter gene transactivation and a full agonist of progesterone receptor induction in MCF-7 cells, thus showing cell- and response-specific differences in the effects of this bivalent ligand. These bivalent ligands for ER do not show enhanced potency or receptor binding affinity: however, some of them display binding properties that suggest the possibility of structure-specific neg. site-site interaction, and some of them function as quite effective estrogen antagonists. 156926-22-6 156926-24-8
RL: BIOL (Biological study)
(estrogen receptor binding by, antagonist activity in relation to) 156926-22-6 CAPLUS
Benzenepropanoic acid, B-ethyl-4-hydroxy-a-(4-hydroxyphenyl)-, 1,4-butanediyl ester, [aR\*(a'R\*, \beta'S\*), \betaS\*]-(-)(9CI) (CA INDEX NAME)

Rotation (-). Absolute stereochemistry unknown.

156926-24-8 CAPLUS Benzenepropanoic acid,  $\beta$ -ethyl-4-hydroxy- $\alpha$ -(4-hydroxyphenyl)-, 1,4-butanediyl ester,  $\{\alpha R^*(\alpha^*R^*,\beta^*S^*),\beta S^*\}$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

ANSWER 59 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

156840-31-2 156840-32-3 156840-33-4
156840-34-5 156840-35-6 156840-36-7
156840-37-8 156840-38-9 156840-39-0
RL: BIOL (Biological Study)
(estrogen receptor binding by, bivalent analogs in relation to)
156840-31-2 CAPLUS
Benzenepropanoic acid, β-ethyl-4-hydroxy-a-(4-hydroxyphenyl)-,
ethyl ester, (R\*,S\*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

156840-32-3 CAPLUS Benzenepropanoic acid,  $\beta$ -ethyl-4-hydroxy- $\alpha$ -{4-hydroxyphenyl}-, butyl ester, (R\*,S\*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

156840-33-4 CAPLUS Benzenepropanoic acid,  $\beta$ -ethyl-4-hydroxy- $\alpha$ -(4-hydroxyphenyl)-, octyl ester, (R\*,S\*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L4 ANSWER 59 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

156840-42-5 156926-25-9 RL: BIOL (Biological study) (estrogen receptor binding by, biol. activity in relation to) 156840-42-5 CAPLUS Benzenepropanoic acid,  $\beta$ -ethyl-4-hydroxy- $\alpha$ -(4-hydroxyphenyl)-, 1,8-octanediyl ester, [aR\*(a'R\*, $\beta$ 'S\*), $\beta$ S\*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

156926-25-9 CAPLUS Benzenepropanoic acid,  $\beta$ -ethyl-4-hydroxy- $\alpha$ -(4-hydroxyphenyl)-, 1,8-octanediyl ester, [aR\*(a'S\*, $\beta$ 'R\*), $\beta$ R\*]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

ANSWER 59 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

156940-34-5 CAPLUS Benzenepropanoic acid, β-ethyl-4-hydroxy-α-(4-hydroxyphenyl)-, 4-hydroxybutyl ester, (R\*,S\*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

156840-35-6 CAPLUS Benzenepropanoic acid,  $\beta$ -ethyl-4-hydroxy- $\alpha$ -(4-hydroxyphenyl)-,  $\theta$ -hydroxyoctyl ester,  $(R^*, S^*)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

156840-36-7 CAPLUS
Benzenepropanoic acid, \$\text{\$\text{\$\text{\$P\$}}\$-\$\text{\$\

Relative stereochemistry.

RN 156840-37-8 CAPLUS

ANSWER 59 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Contine Benzenepropanoic acid, \$-ethyl-4-hydroxy-a-(4-hydroxyphenyl)-, 2-(2-ethoxyethoxy)ethyl ester, (R\*,S\*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

156840-38-9 CAPLUS Benzenepropanoic acid,  $\beta$ -ethyl-4-hydroxy- $\alpha$ -(4-hydroxyphenyl)-, 2-(2-hydroxyethoxy)ethyl ester,  $(R^*,S^*)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

156840-39-0 CAPLUS Benzenepropanoic acid,  $\beta$ -ethyl-4-hydroxy- $\alpha$ -(4-hydroxyphenyl)-, 2-[2-(2-hydroxyethoxy)ethoxy]ethyl ester,  $(R^*,S^*)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

ANSWER 59 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

156840-41-4 CAPLUS Benzenepropanoic acid,  $\beta$ -ethyl-4-hydroxy- $\alpha$ -(4-hydroxyphenyl)-, 1,3-propanediyl ester, [ $\alpha$ R'( $\alpha$ 'R', $\beta$ 'S'), $\beta$ S']- (9CI) (CA INDEX NAME)

Relative stereochemistry.

156840-47-0 CAPLUS Benzenepropanoic acid,  $\beta$ -ethyl-4-hydroxy- $\alpha$ -(4-hydroxyphenyl)-, oxydi-2,1-ethanediyl ester,  $\{\alpha R^*(\alpha^*R^*,\beta^*S^*),\beta S^*\}$ -(9CI) (CA INDEX NAME)

Relative stereochemistry.

ANSWER 59 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN ethyl ester, (R\*,R\*)- (9CI) (CA INDEX NAME) (Continued)

Relative stereochemistry.

156840-30-1 CAPLUS Benzenepropanoic acid,  $\beta$ -ethyl-4-hydroxy- $\alpha$ -(4-hydroxyphenyl)-, 1,4-butanediyl ester, [ $\alpha$ R\*( $\alpha$ 'R\*, $\beta$ 'S'), $\beta$ S\*]-(+)-(9CI) (CA INDEX NAME)

Rotation (+). Absolute stereochemistry unknown.

156840-40-3 CAPLUS Benzenepropanoic acid,  $\beta$ -ethyl-4-hydroxy- $\alpha$ -(4-hydroxyphenyl)-, l,2-ethanediyl ester, [aR'(a'R',\beta'S'),\betaS\*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

ANSWER 59 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

156840-48-1 CAPLUS Benzenepropanoic acid,  $\beta$ -ethyl-4-hydroxy- $\alpha$ -(4-hydroxyphenyl}-1,2-ethanediylbis(oxy-2,1-ethanediyl) ester,  $[\alpha R^*(\alpha^*R^*,\beta^*S^*)]$ -(9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-B

156840-49-2 CAPLUS Benzenepropanoic acid, \(\text{\$\text{\$\text{\$P\$-ethyl-4-hydroxy-\$\text{\$\

Relative stereochemistry.

PAGE 1-B

156840-50-5 CAPLUS Benzenepropanoic acid,  $\beta$ -ethyl-4-hydroxy- $\alpha$ -(4-hydroxyphenyl)-, 3,6,9,12-tetraoxatetradecane-1,14-diyl ester, [ $\alpha$ R\*( $\alpha$ 'R\*, $\beta$ 'S\*), $\beta$ S\*]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L4 ANSWER 59 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN oxydi-2,1-ethanediyl ester, [aR\*(a\*5\*,β\*R\*),βR\*]-(9CI) (CA INDEX NAME)

Relative stereochemistry.

156926-29-3 CAPLUS Benzenepropanoic acid,  $\beta$ -ethyl-4-hydroxy- $\alpha$ -(4-hydroxyphenyl)-, 1,2-ethanedlylbis (oxy-2,1-ethanedlyl) ester, [aR\*(a\*S\*, $\beta$ \*R\*), $\beta$ R\*]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-B

156926-30-6 CAPLUS Benzenepropanoic acid,  $\beta$ -ethyl-4-hydroxy- $\alpha$ -(4-hydroxyphenyl)-, oxybis(2.1-ethanediyl)cxy-2,1-ethanediyl) ester, [=R\*( $\alpha$ 'S\*, $\beta$ 'R\*), $\beta$ R\*]- (9C1) (CA INDEX NAME)

L4 ANSWER 59 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN

(Continued)

PAGE 1-A

PAGE 1-B

156926-23-7 CAPLUS Benzenepropanoic acid,  $\beta$ -ethyl-4-hydroxy- $\alpha$ -(4-hydroxyphenyl)-, 1.4-butanediyl ester, [ $\alpha R^*(\alpha^*S^*,\beta^*R^*),\beta R^*$ ]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

156926-28-2 CAPLUS Benzenepropanoic acid,  $\beta$ -ethyl-4-hydroxy- $\alpha$ -(4-hydroxyphenyl)-,

L4 ANSWER 59 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN Relative stereochemistry. (Continued)

PAGE 1-A

PAGE 1-B

156926-31-7 CAPLUS Benzenepropanoic acid,  $\beta$ -ethyl-4-hydroxy- $\alpha$ -(4-hydroxyphenyl)-, 3,6,9,12-tetraoxatetradecane-1,14-diyl ester, [ $\alpha$ N' ( $\alpha$ 'S', $\beta$ 'N'), $\beta$ N']- (9C1) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A

ANSWER 59 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) PAGE 1-B

ANSWER 61 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1994:269805 CAPLUS 120:269805

120:269805
Scope and mechanism of the reaction of alkylidenephosphoranes with
10-methyleneanthrone
Ganoub, Neven A. F.; Abdou, Wafaa M.; Yakout, El Sayed M. A.
Dep. Pestic. Chem., Natl. Res. Cent., Cairo, Egypt
Phosphorus, Sulfur and Silicon and the Related Elements (1993), 84 (1-4),
197-204
CODEN: PSSLEC: ISSN: 1042-6507

Journal English

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

Quinone methide I reacts with excess (carbomethoxymethylene)triphenylphosp horane to afford bisanthracenol II (R = COZMe), III (R1 = Me), and ylides IV and V; reaction of I with (carbethoxymethylene)triphenylphosphorane gave similar and different products. The polarity of the solvent had a limited effect on the reaction. Mechanistic studies suggest that I can react as a Diels-Alder diene and function as a dienophile in the same reaction. Wittig reactions of IV and V with BzH were described. 154504-11-7P
RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and Wittig reaction with benzaldehyde) 154504-11-7 CAPLUS
9-Anthracenepropanoic acid, 10-[1-{(10-hydroxy-9-anthracenyl)methyl]-2-methoxy-2-coxoethyl]-a-(triphenylphosphoranylidene)-, methyl ester (9CI) (CA INDEX NAME)

154504-14-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
154504-14-0 CAPUS
9-Anthracenepropanoic acid, 10-[1-[(10-hydroxy-9-anthracenyi)methyl]-2-methoxy-2-oxoethyl]-α-(phenylmethylene)-, methyl ester (9CI) (CA
INDEX NAME)

ANSWER 60 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1994:270919 CAPLUS 120:270919

120:270919
Synthesis of saulatine
Kim, Dong Chin: Yoon, Won Hyung: Choi, Hoon: Kim, Dong H.
Dep. Chem., Pohang Inst. Sci. Technol., Pohang, 790-600, S. Korea
Journal of Heterocyclic Chemistry (1993), 30(5), 1431-6
CODEN: JHTCAD: ISSN: 0022-152X

Journal English CASREACT 120:270919

A study directed toward the synthesis of saulatine (5,8,9,14a-tetrahydro-3,4,11,12-tetramethoxyisoquino[1,2-b]benzazepine-6,14-dione) ([] is described. The successful synthetic route consists of three steps starting with 3,4-dimethoxyphenethylamine and 2-bromo-(3,4-dimethoxy-2-ethoxycarbomethylphenyl) acetate. The methoxy moieties present on the aromatic rings prohibit the use of the intramol. Friedel-Crafts reaction

ΙT

a Lewis acid catalyst for ring construction because of their demethylation tendency under the reaction conditions.
154534-99-3P
RL: PREP (Preparation)
(intermediate in attempted synthesis of saulatine)
154534-99-3 CAPLUS
Butanedioic acid, 2,3-bis(2-bromo-4,5-dimethoxyphenyl)-, diethyl ester
(9CI) (CA INDEX NAME)

ANSWER 61 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

L4	ANSWER 62 OF 146 C	APLUS	COPYRIGHT 2	007 ACS on STN	
AN	1994:163733 CAPLUS				
DN	120:163733				
ΤI		e insec	ticides and	or acaricides conta	ining the same
	active ingredient a	nd inte	rmediate co	mpounds thereof	•
IN	Taki, Toshiaki: Kis	ida. Hi	rosi: Saito	, Shigeru: Isayama,	Shinii
PA					
50	Eur. Pat. Appl., 96				
	CODEN: EPXXDW	PP.			
DT					
LA	English				
	CNT 1				
	PATENT- NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 567138	A2	19931027	EP 1993-106584	19930422
	EP 567138				
	R: CH, DE, ES,			ı.	
	CA 2094333	Al	19931024	CA 1993-2094333	19930419
	US 5451607	A	19950919		19930419
	JP 06056754				
	BR 9301628		19931026		
	AU 9337063	Ä	19931028		
		B2	19950302	1333 3.003	13330422
DDAT	JP 1992-131616		19920423		
os	MARPAT 120:163733		13320423		
GI	HANNAN ILV:103133				

The title compds. I [A = (CH2)t, O, S(O)n, OCH2, (un)substituted NH, etc.; n = 0-2; t = 1-3; R1 = halogen, CN, NO2, azide, etc.; R2 = H, C1-6 alkyl, C1-6 haloalkyl, C3-6 cycloalkyl, C2-6 alkenyl, (un)substituted Ph, etc.; R3 = H, C1-6 alkyl, C1-6 haloalkyl, C2-6 alkenyl, C2-6 haloalkenyl, C2-6 alkynyl, etc.; R4 = H, C1-6 alkyl, C1-6 haloalkyl; R5 = C1-6 alkyl, C1-6 haloalkyl; C2-6 alkenyl, C2-6 alkenyl, C2-6 alkyl, C1-6 haloalkyl; R5 = C1-6 alkyl, C1-6 haloalkyl; C2-6 alkenyl, C2-6 alkenyl, C2-6 alkynyl, etc.; R6 = H, C1-6 alkyl, C2-6 alkenyl, C2-6 alkenyl, C2-6 alkynyl, etc.; R6 = H, C1-6 alkyl, C2-6 alkenyl, C2-6 alkenyl, C2-6 alkynyl, etc.; R6 = H, C1-6 alkyl, C2-6 alkenyl, C2-6 alkenyl, C2-6 alkynyl, etc.; R6 = H, C1-6 alkyl, C2-6 alkenyl, C2-6 alkenyl, C2-6 alkynyl, etc.; R6 = H, C1-6 alkyl, C2-6 alkenyl, C2-6 alkenyl, C2-6 alkynyl, etc.; R6 = H, C1-6 alkyl, C1-6 a

L4	ANSWER 63 OF 146 C	CAPLUS COPYRIGHT	2007 ACS on STN			
AN	1994:134276 CAPLUS					
DN	120:134276					
TI	Agrochemical arthro	opodicidal amides				
IN			d: March, Robert William,	, Jr.		
PA	du Pont de Nemours,		USA			
50	PCT Int. Appl., 129	9 pp.				
	CODEN: PIXXD2					
DT	Patent					
LA	English	•				
FAN.	CNT 1					
	PATENT NO.	KIND DATE	APPLICATION NO.	DATE		
			APPLICATION NO.			
PΙ	WO 9319045	A1 19930930	WO 1993-US2434	19930318		
			JP, KP, KR, KZ, LK, MG,	MN, MW, NO,		
		, RU, SD, SK, UA,				
			GB, GR, IE, IT, LU, MC,			
	BF, BJ, CF,	, CG, CI, CM, GA,	GN, ML, MR, SN, TD, TG			
	AU 9338118	A 19931021	AU 1993-38118 EP 1993-907555	19930318		
	EP 632803	A1 19950111	EP 1993-907555	19930318		
	EP 632803					
	R: ES, FR, IT					
	JP 07507276	T 19950810		19930318		
	JP 3446052	B2 20030916				
	BR 9306225	A 19980630		19930318		
	ES 2127270	T3 19990416				
	CN 1098093	A 19950201				
	US 5514678 US 1992-858205	A 19960507		19940922		
PRAI	US 1992-858205	A2 19920326				
	US 1992-875174					
	WO 1993-US2434	A 19930318				
OS GI	MARPAT 120:134276					
61						

AB The title compds. QC(:X)N(Y)G [G = (un)substituted pyridyl, (un)substituted Ph, (un)substituted cyclohexyl, (un)substituted piperidino; Q = phenyldihydropyrrolyl, phenylheterocyclyl, etc., X = 0, 5; Y = H, C1-6 alkyl, PhCH2, C2-6 alkenyl, C2-6 alkenyl, C2-6 alkenyl, c2-6; useful for the control of arthropods in both agronomic and nonagronomic environments, are prepared and their activity is demonstrated against a wide variety of arthropod species. Thus, dihydropyrrole I (n.p. 200-201°) was prepared

17 152628-91-6P
RL: RCT (Reactant): SPN (Synthetic preparation): PREP (Preparation): RACT (Reactant or reagent) (preparation and reaction of, in preparation of agrochem.
arthropodicidal anides)
RN 152628-91-6 CAPUS
CN Benzenepropanoic acid, 4-chloro-α-(4-chlorophenyl)-β-(nitromethyl)-, methyl ester (CA INDEX NAME)

ANSWER 62 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
153278-90-1P
RL: RCT (Reactant): SPN (Synthetic preparation): PREP (Preparation): RACT
(Reactant or reagent)
(preparation and reaction of, in preparation of hydrazone insecticides)
153278-90-1 CAPLUS
Benzenepropanoic acid, 3-chloro-α-(4-chlorophenyl)-, ethyl ester
(CA INDEX NAME)

ANSWER 63 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN

ANSWER 64 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN
1993:494855 CAPLUS
119:94855
Laser Raman spectroscopic study on two isomers of a-polysubstituted dibenzyl compounds
Qi, Chenzer Zhang, Bin; Jia, Xueqing; Yang, Dilun
Dep. Chem., Lanzhou Univ., Lanzhou, 730000, Peop. Rep. China
Guangpusue Yu Guangpu Fenxi (1992), 12(4), 11-14
CODEN: GYGFED; ISSN: 1000-0593
JOURNAL
COLEN: GYGFED; ISSN: 1000-0593
JOURNAL
Chinese
Five pairs of meso- and dL-4-XCGH4C(CN) (CO2Et)C(CN) (CO2Et)CGH4X-4 (X = H, Cl, Me, MeO, NO2) have been studied by laser Raman spectroscopy. The
Raman bands of some groups have been analyzed. The effect of different
configurations on the laser Raman spectra is discussed.
139257-67-3 139257-68-4 139257-70-8
139257-67-3 139257-68-4 139257-70-8
139257-67-3 CAPLUS
Butanedioic acid, 2, 3-dicyano-2,3-bis(4-methylphenyl)-, diethyl ester,
(2R, 35)-rel- (9CI) (CA INDEX NAME)

#### Relative stereochemistry.

139257-68-4 CAPLUS Butanedioic acid, 2,3-dicyano-2,3-bis(4-methylphenyl)-, diethyl ester, (2R,3R)-rel- (9CI) (CA INDEX NAME)

139257-70-8 CAPLUS Butanedioic acid, 2,3-bis(4-chlorophenyl)-2,3-dicyano-, diethyl ester, (ZR,35)-rel- (9C1) (CA INDEX NAME)

ANSWER 65 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1993:491499 CAPLUS 119:91499 Effect of molecular configuration and substituent electronic effect on carbon-13 NMR spectra of diethyl 2,3-dicyano-2,3-bis(p-substituted phenyl)succinates Yang, Dilun; Qi, Chenze: Wu, Jingjiar Cui, Yuxin: Liu, Youcheng Dep. Chem., Lanzhou Univ., Lanzhou, 730000, Peop. Rep. China Gaodeng Xuexiao Huaxue Xuebao (1993), 14(2), 257-60 COUDE: KTHPUM: ISSN: 0251-0790 Journal Chinese

$$x - \left( \begin{array}{c} CN \\ \frac{1}{C} \\ \frac{1}{CO_{2}Et} \\ \frac{1}{CO_{2}Et} \end{array} \right) - X$$

The meso (I: X = OCH3, CH3, H, Cl, NO2) and dL isomers (II: same X) of the title esters are studied by 13C NMR spectrometry. The chemical shifts of

carbon atoms in the same group on both sides of the central C-C bond are equivalent, and the chemical shifts of the C7-C9 atoms in II are smaller in

In I. Plots of chemical shifts of C6, C7 and C8 atoms vs. Hammett o consts. of substituents in the para position of the benzene ring are

Construction of the benzene ring are linear.

139257-67-3 139257-68-4 139257-70-8 139257-71-9 RL: PRP (Properties) (carbon-13 NNR of) 139257-67-3 CAPLUS Butanedioic acid, 2,3-dicyano-2,3-bis(4-methylphenyl)-, diethyl ester, (2R,35)-rel- (9CI) (CA INDEX NAME)

#### Relative stereochemistry.

139257-68-4 CAPLUS
Butanedioic acid, 2,3-dicyano-2,3-bis(4-methylphenyl)-, diethyl ester,

L4 ANSWER 64 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

139257-71-9 CAPLUS Butanedioic acid, 2,3-bis(4-chlorophenyl)-2,3-dicyano-, diethyl ester, (2R,3R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

ANSWER 65 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (2R,3R)-rel- (9CI) (CA INDEX NAME) (Continued)

#### Relative stereochemistry.

139257-70-8 CAPLUS Butanedioic acid, 2,3-bis(4-chlorophenyl)-2,3-dicyano-, diethyl ester, (ZR,35)-cel- (9CI) (CA INDEX NAME)

#### Relative stereochemistry.

139257-71-9 CAPLUS Butanedioic acid, 2,3-bis(4-chlorophenyl)-2,3-dicyano-, diethyl ester, (ZR,JR)-rel- (9CI) (CA INDEX NAME)

#### Relative stereochemistry.

ANSWER 66 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1993:408231 CAPLUS 119:8231

119:8231
Study on the mechanism of oxidative coupling reactions of ethyl a-cyano-p-X-substituted phenylacetates by using the catalyst [Cu2\*(OH-)TMED)2C12
Yang, Dilun: Qi, Chenze: Lu, Minglan: Liu, Youcheng
Dep. Chem., Lanzhou Univ., 730000, Peop. Rep. China
Huaxue Xuebao (1993), 51(1), 66-72
CODEN: HHHPA4: ISSN: 0567-7351

DT LA GI

ŧ,

$$x \longrightarrow \begin{matrix} c_{N} \\ c_{HCO2Et} \end{matrix} \qquad x \longrightarrow \begin{matrix} c_{N} \\ c_{O2Et} \\ c_{O2Et} \end{matrix} \begin{matrix} c_{CO2Et} \\ c_{O2Et} \end{matrix} \begin{matrix} c_{CO2Et} \\ c_{O2Et} \end{matrix}$$

The oxidative coupling reactions of the title compds. I (X = OCH3, CH3, H, Cl, NO2) with Cu2+-TMEDA-O2 (TMEDA = N,N,N',N'-tetramethylenediamine) system give meso- and dl-succinates II. On the basis of the stereochem. and IR, IH NMR and EPR determination of the reactive intermediates of the oxidative coupling reactions, the mechanism was suggested.

139257-61-3P 139257-68-4P 139257-70-8P

139257-71-9P
RL: SPN (Synthetic preparation): PREP (Preparation)
(preparation of)
139257-61-3 CAPLUS
Butanediot acid, 2,3-dicyano-2,3-bis(4-methylphenyl)-, diethyl ester,
(2R,35)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

139257-68-4 CAPLUS Butanedioic acid, 2,3-dicyano-2,3-bis(4-methylphenyl)-, diethyl ester, (ZR,3R)-rel (9CI) (CA INDEX NAME)

Relative stereochemistry.

DT LA FAN.

DATE PI JP 05009246 A 19930119 JP 1991-160844 19910606
PRAI JP 1991-160844 19910606
AB The title products are manufactured by curing prepreg materials containing

The title products are manufactured by curing prepreg materials containing std.

polyesters or vinyl ester resins in the presence of R3C6H4CR1R2CR1R2C6H4R3 (R1 = cyano, CO2Me, CO2Et: R2 = CO2Me, CO2Et: R3 = H, Me, OMe) at 60-100°. Thus, a glass mat was was impregnated with a composition containing Polylite 8010 100, NS 100 100, 1,2-bis(p-methoxyphenyl)-1,2-dicarboethoxy-1,2-dicyanoethane 1, Zn stearate 4, and Mg0 0.5 part, sandwiched between polyethylene films, and kept at 20° for 7 days to give a prepreg mat showing gelation time >180 days at 20° and giving cured product with Barcoll hardness 60.

31249-03-3 34404-72-3, 1,2-Bis(p-methylphenyl) tertacarboenthoxyethane 70230-43-2

147992-58-3 147992-59-4 147992-60-7,

1,2-Bis (p-methylphenyl) tetracarboenthoxyethane

RL: CAT (Catalyst use): USES (Uses)

(catalysts, unsatd. polyesters and vinyl ester resins containing, for prepregs with long shelf life)

31249-03-3 CAPLUS

Butanedioic acid, 2,3-dicyano-2,3-bis(4-methylphenyl)-, dimethyl ester (9C1) (CA INDEX NAME)

34404-72-3 CAPLUS
1,1,2,2-Ethanettracarboxylic acid, 1,2-bis(4-methylphenyl)-, tetramethyl ester (9CI) (CA INDEX NAME)

ANSWER 66 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN

(Continued)

139257-70-8 CAPLUS Butanedioic acid, 2,3-bis(4-chlorophenyl)-2,3-dicyano-, diethyl ester, (ZR,35)-cel-(9CI) (CA INDEX NAME)

Relative stereochemistry.

Relative stereochemistry.

139257-71-9 CAPLUS Butanedioic acid, 2,3-bis(4-chlorophenyl)-2,3-dicyano-, diethyl ester, (2R,3R)-rel- (9CI) (CA INDEX NAME)

ANSWER 67 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

70230-43-2 CAPLUS Butanedioic acid, 2,3-dicyano-2,3-bis(4-methylphenyl)-, 1,4-diethyl ester (CA INDEX NAME)

147992-58-3 CAPLUS Butanedioic acid, 2,3-dicyano-2,3-bis(2,4-dimethylphenyl)-, diethyl ester (9C1) (CA INDEX NAME)

147992-59-4 CAPLUS Butanedioic acid, 2,3-dicyano-2,3-bis(2,4-dimethylphenyl)-, dimethyl ester (9C1) (CA INDEX NAME)

147992-60-7 CAPLUS 1.1.2,2-Ethanetetracarboxylic acid, 1,2-bis(4-methylphenyl)-, tetraethyl ester (9C1) (CA INDEX NAME)

ANSWER 67 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

$$\mathsf{Me} = \underbrace{\begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}}_{\mathsf{EtO}-\mathsf{C}} \underbrace{\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}}_{\mathsf{Ne}} \mathsf{Me}$$

4

L4 ANSWER 68 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

139257-70-8 CAPLUS Butanedioic acid, 2,3-bis(4-chlorophenyl)-2,3-dicyano-, diethyl ester, (ZR,35)-cel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

139257-71-9 CAPLUS Butanedioic acid, 2,3-bis(4-chlorophenyl)-2,3-dicyano-, diethyl ester, (ZR,3)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

ANSWER 68 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1993:22683 CAPLUS 118:22683 CAPLUS 118:22683 Synthesis of diethyl 2,3-dicyano-2,3-bi(p-substituted phenyl)succinates and its decomposition in styrene Yang, Dilun; Qi, Chenze: Li, Zhaolong: Liu, Youcheng Dep. Chem., Lanzhou Univ., Lanzhou, 730000, Peop. Rep. China Gaodeng Xuexiao Huaxue Xuebao (1991), 12(12), 1623-6 CODEN: KTHPON: ISSN: 0251-0790 Journal Chinese CASREACT 118:22683 Di-Et 2,3-dicyano-2,3-bis(p-X-phenyl)succinates (X = MeO, Me, Cl, NO2) were prepared by oxidative coupling of the corresponding Et (cyanophenyl)acetates, and their meso and dl isomers were separated and characterized by proton NMR, IR, x-ray, and mass spectroscopy. The thermal decomposition rates of the meso-isomers of these succinates in DT LA OS AB

styrene
at 100° were greater than those of the d1-isomers except for the
isomer with X = MeO. The substituent effect on the thermal decomposition

of these succinates followed the order: MeO > Me > Cl > H.
139257-67-3P 139257-68-4P 139257-70-8P
139257-17-9P
RL: RCT (Reactant): PREF (Preparation): RACT (Reactant or reagent)
(synthesis and decomposition of)
139257-67-3 CAPLUS
Butanedioic acid, 2, 3-dicyano-2, 3-bis(4-methylphenyl)-, diethyl ester,
(2R, 3S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

139257-68-4 CAPLUS Butamedioic acid, 2,3-dicyano-2,3-bis(4-methylphenyl)-, diethyl ester, (ZR,R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

ANSWER 69 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1993:21868 CAPLUS 118:21868

AN DN TI

118:21868
Studies on the proton NMR spectra of meso and dl diethyl
2,3-dicyano-2,3-bis(p-substituted phenyl)succinates
Yang, Dilun; Qi, Chenzer Cui, Yuxin; Dang, Haishan; Liu, Youcheng
Dep. Chem., Lanzhou Univ., Lanzhou, 730000, Peop. Rep. China
Gaodeng Xuexiao Huaxue Xuebao (1991), 12(12), 1627-30
CODEN: KTHEPM: 15SN: 0251-0790

AU CS SO

Journal Chinese

DT LA AB The IH NMR of meso- and dl-diethyl 2,3-dicyano-2,3-di(p-X-phenyl) succinates (X = OCH3, CH3, H, Cl, NO2) and IH Noesy spectra of meso- and dl-isomers of the di-Et ester with X = CH3 were determined by using a

di-isomers of the di-Et ester with X = CH3 were determined by using a Bruker AM

400 MHz superconducting NMR spectrometer. The corresponding proton of the substituent groups attached to the two central C atoms in the mols. are chemical shift equivalence. The average difference between o-IH absorptions of

Ph in the dl-isomers and that in meso-isomers was found to be .hivin.A5dl-meso = -120.1 ± 6.1 Hz. All of the meso-isomers, then, have methylene (ABX3 system) and Me in the ethoxy at upfield positions, and all of the dl-isomers have that at downfield positions. hivin.A5dl-meso = 53.3 ± 5.9 Hz and .hivin.D4dl-meso = 53.5 ± 5.9 Hz and .hivin.D4dl-meso = 53.5 ± 5.9 Hz and .hivin.A5dl-meso = 53.5 ± 5.9 Hz for protons in the methylenes, and .hivin.D4dl-meso = 39.3 ± 3.5 Hz for protons in the methyls. .hivin.A5dl-meso Is the mark of influence of mol. configuration on the chemical shift.

IT 139257-67-3 139257-68-4 139257-70-8 139257-71-9 RL: PRF (Properties)

139257-71-9

(proton NMR of, monoequivalents of methylene group in)
139257-67-3 CAPLUS
Butanedioic acid, 2,3-dicyano-2,3-bis(4-methylphenyl)-, diethyl ester,
(2R,3S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

139257-68-4 CAPLUS Butanedioic acid, 2,3-dicyano-2,3-bis(4-methylphenyl)-, diethyl ester, (ZR,3R)-cel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

ANSWER 69 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN

8

139257-70-8 CAPLUS Butanedioic acid, 2,3-bis(4-chlorophenyl)-2,3-dicyano-, diethyl ester, (2R,3S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

139257-71-9 CAPLUS Butanedioic acid, 2,3-bis(4-chlorophenyl)-2,3-dicyano-, diethyl ester, (ZR,3R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

ANSWER 70 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

144633-01-2 CAPLUS
Butanedicic acid, 2,3-bis[3,5-bis(trifluoromethyl)phenyl]-, diethyl ester, (R\*,5\*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

144633-02-3 CAPLUS Butanedio (dic acid, 2,3-bis[4-(trifluoromethyl)phenyl]-, diethyl ester, (RY.51)- (9C1) (CA INDEX NAME)

Relative stereochemistry.

144633-04-5 CAPLUS Butanedioic acid, 2,3-bis{2-(trifluoromethyl)phenyl}-, diethyl ester,  $(R^*,R^*)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

ANSWER 70 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1992:651025 CAPLUS 117:251025 Electrochemistry of ethyl a-bromo-a-fluoro(phenyl)acetate and some ethyl a-bromo(trifluoromethylphenyl)acetates and electrochemical synthesis of the corresponding diastereoisomeric diethyl succidates succinates Succinates Mattiello, Leonardo; Rampazzo, Liliana; Sotgiu, Giovanni Dip. ICMNPM, Univ. Roma 'La Sapienza', Rome, 00161, Italy Journal of Chemical Research, Synopses (1992), (10), 321 CODEN: JRPSDC; ISSN: 0308-2342

Electrolysis of PhCFBrCO2Et and title bromo(trifluoromethyl)phenylacetates 1 (R1 = CF3, R2-R4 = H: R1 = R3 = R4 = H, R2 = CF3, R1 = R3 = H, R2 = R4 = CF3) n reticulated vitreous carbon in DMF gave diners PhCF(COZET)CF(COZET)Ph and II. II were obtained as mixture of meso- and DL-forms. 14652-99-5P, 144633-00-1P 144633-01-2P 144633-02-3P 144633-07-8P R4653-07-8P R4653-07-8P R4653-07-8P R4653-07-8P R4653-07-8P R4653-07-8P R4653-05-6P R4653-05-07 14653-07-8P R4653-07-8P R46

Relative stereochemistry.

144633-00-1 CAPLUS Butanedioic acid, 2,3-bis[3-(trifluoromethyl)phenyl]-, diethyl ester, (%,5:)- (9C1) (CA INDEX NAME)

Relative stereochemistry.

ANSWER 70 OF 146 CAPLUS COPYRIGHT 2007 ACS ON STN (Continued)

144633-05-6 CAPLUS Butanedioic acid, 2,3-bis[3-(trifluoromethyl)phenyl]-, diethyl ester, (R\*,R\*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

$$F_3C \xrightarrow{\text{$\mathbb{R}$ $\mathbb{R}$ }} \mathbb{R}^{\text{$\mathbb{R}$ }}$$

144633-06-7 CAPLUS Butanedioic acid, 2,3-bis(3,5-bis(trifluoromethyl)phenyl]-, diethyl ester, (Rr.R1)- (9C1) (CA INDEX NAME)

Relative stereochemistry.

144633-07-8 CAPLUS Butanedioic acid, 2,3-bis[4-(trifluoromethyl)phenyl}-, diethyl ester, (R\*,R\*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

ANSWER 70 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN

ANSWER 71 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) (halo) alkynyl, C3-6 (halo) cycloalkyl, halo, cyano, N3, etc. or R2R2 - CXH2O, OCF2O, OCH2CH2O, etc.; R3 = H, N3, N02, halo, C1-6 (halo) alkyl, c2-6 alkenyl, (substituted) Ph, etc.; R4, R5 = H, C1-4 alkyl, etc.; R4R5 - O, S; R8 = (substituted) C1-3 alkyl, C2-4 (halo) alkenyl, (substituted) benzyl, etc.; R9 = H, C1-4 alkyl, C1-4 haloalkyl, C2-4 alkoxycarbonyl, (substituted) Ph, -pyridyl or R8R9 = (CH2)4, (CH2)5, etc.; R31 = H, C1-4 alkyl, C2-4 alkanyl, C2-4 alkoxycarbonyl) were prepd. for use in controlling anthropods, e.g. insects, pests, acari, etc. Thus, 5-chloro-2-(4-chlorophenyl)-2,3-dihydro-2-hydroxy-Hi-inden-1-one (prepn. given) was treated with hydrazine then 4-CF3CGHANCO to give hydrazinearboxamide III. The latter was cyclized with CH2O and TosOH to give title compd. IV. IV at 0.55 kg/ha gave ≥80% control of Spodoptera fruigiperda on wheat germ.

144172-20-3P
RL: SPN (Synthetic preparation); PREF (Preparation)

144172-20-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of, as intermediate for arthropodicides)
144172-20-3 CAPLUS
Benzenepropanoic acid, 3-chloro-α-(4-chlorophenyl)-, methyl ester
(CA INDEX NAME)

ANSWER 71 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1992:634026 CAPLUS 117:234026 Preparation of indenooxadiazinecarboxamides as arthropodicides Annis, Gaty David; Barnette, William Eldo; McCann, Stephen Frederick; Wing, Keith Dumont du Font de Nemours, E. I., and Co., USA PCT Int. Appl., 351 pp. CODEN: PIXX02 Patent English CNT 1 PA SO LA En FAN.CNT ONT 1 PATENT NO. 1993011
1 1993011
1 19950802
EP 1992-902235
1 19911217
B1 19950802
ED, DK, ES, FR, GB, GR, IT, LI, LU, MC, NL, SE
A2 19940502
HU 1993-1808
F 19970828
T 19940602
T 19940602
T 19940602
T 19940614
ER 1991-7246
19911217
T3 19951116
ES 1992-902235
19911217
C1 19971120
RU 1991-5011055
19911217
A 19930612
A 19930612
A 19930621
B 19970409
A 19951031
US 1993-75534
A 19980113
US 1993-75534
19930618
A 19980111
A 19991021
A2 19910611
A 1991021
A3 19930618 565574 19931020 EP 1992-902235 19911217 EP 565574 R: AT, BE, CH, DE, HU 65223 A HU 65223 JP 06504777 BR 9107246 ES 2077392 RU 2096409 IL 100429 CN 1062726 CN 1034468 US 546293 US 5708170 US 1990-632438 US 1991-714401 US 1991-714401 US 1993-75534 US 1993-75534 PRAI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

Title compds. QC(:X)NYG and QX1C:NG [I and II; Q = Q1, Q2, etc.; A = H; E = H, C1-3 alkyl or AE = CH2, CH2CH2, O, S, SO, SO2, OCH2, SCH2, etc.; G = (substituted) Ph, -pyridyl, -pyrimidyl, -thienyl, etc.; X = O, S, NX2; X1 = C1, Br, OR8, SR8, NR8R9: X2 = R8, OH, OR8, cyano, SOZR8, SOZPh, etc.; Y = H, C1-6 (halo)alkyl, CH2Ph, C2-6 alkoxyalkyl, C2-6 alkenyl, C2-6 alkynyl, C1-3 alkoxy, cyano, NO2, (substituted) Ph, etc.; Z = C, N: Z1 = O, S, NR31; R2 = H, (substituted) C1-6 alkyl, C2-6 (halo) alkenyl, C2-6

so

ANSWER 72 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1992:625501 12012:25501 1201

Relative stereochemistry.

Relative stereochemistry.

139257-68-4 CAPLUS Butamedioic acid, 2,3-dicyano-2,3-bis(4-methylphenyl)-, diethyl ester, (ZR,3R)-est-(9CI) (CA INDEX NAME)

ANSWER 73 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1992:448048 CAPLUS 117:48048 Electrochemical methoxylation of arylacetates Kato, Mitsukor Suzuki, Shohei: Shimamura, Miyako: Nozawa, Koohei: Kawai, Kenichi: Nakajima, Shoichi Fac. Pharm. Sci., Hoshi Univ., Tokyo, 142, Japan Chemical & Pharmaceutical Bulletin (1992), 40(4), 1037-8 CODEN: CPRTAL: ISSN: 0009-2363 Journal English

Journal English CASREAT 117:48048 Electrochem. methoxylation at the active methylene group of phenylacetates and 1-naphthaleneacetate was conducted successfully at room temperature in methanol containing potassium iodide as electron carrier and sodium notice.

methoxide
as base and methoxylating agent. Along with the monomethoxylated
products, dimethoxy, hydroxy, and oxo derivs. as well as the dimers
(succinates) were produced as byproducts.

IT 12472-20-6P

142472-20-6P
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, in electrochem. methoxylation of Me arylacetate)
142472-20-6 CAPLUS
Butanedoic acid, 2,3-bis(4-chlorophenyl)-, dimethyl ester (9CI) (CA
INDEX NAME)

(Continued) ANSWER 74 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN

CRN 139257-68-4 CMF C24 H24 N2 O4

Relative stereochemistry

CM 2

CRN 56-23-5 CMF C C14

139257-70-8 CAPLUS

Butanedioic acid, 2,3-bis(4-chlorophenyl)-2,3-dicyano-, diethyl ester, (2R,3S)-rel- (9CI) (CA INDEX NAME)

139257-71-9 CAPLUS Butanedioic acid, 2,3-bis(4-chlorophenyl)-2,3-dicyano-, diethyl ester, (ZR,3R)-rel- (9CI) (CA INDEX NAME)

ANSWER 74 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1992:117741 CAPLUS 116:117741 CAPLUS 116:117741 and molecular structures of meso- and dl-diethyl 2,3-dicysno-2,3-di [p-substituted phenyl] succinates Yang, Dilun; Ql, Chenze; Zhu, Ying; Wang, Xin; Liu, Youcheng Dep. Chem., Lanzhou Univ., Lanzhou, 730000, Peop. Rep. China Huaxue Xuebao (1991), 49(12), 1457-66 CODEN: HHHPA4; ISSN: 0567-7351 Journal Chinese

Chinese
The crystal and mol. structures of meso- and dl-diethyl
2,3-dicyano-2,3-di(p-X-substituted phenyl) succinates, X:OCH3, meso (I),
dl-l (II): X = CH3 meso-(III):, dl-(IV): X = Cl (V), meso-(VI), dl were
determined I decomposed when its diffraction at a were being collected.

nonoclinic, space group P21/c; final R = 0.0413 for 2488 reflections. III is triclinic space group P.hivin.1; a = final R = 0.0501 for 2191 observed reflections. IV is triclinic, space group P.hivin.1; a = final R = 0.0804 for 3049 observed reflections. V is monoclinic, space group P21/c; a =

for 3049 observed reflections. V is monoclinic, space group P21/c: a = sl

R = 0.0585 for 1460 reflections. VI is monoclinic, space group P21/c: final R = 0.0521 for 2347 reflections. Atomic coordinates are given. In comparison with normal C-C single bond (0.1544 nm), the bond length for the central C-C bond in all of the diastereoisomers shows a remarkable lengthening effect of 0.0023-0.0052 (nm) (1.4-3.41). The bond length for the central bonds in all of meso-isomers is longer than that in corresponding d1-isomers. Among the substituted groups attached to the 2 central C atoms in the mols. of all of the diastereoisomers resp., the interat. distance between nonbonded atoms is smaller than the sum of Van der Waals radii, indicating the existence of secious steric hindrance which is mainly responsible for the lengthening effect.

139257-67-3 139257-69-5 139257-70-8

139257-67-3 CAPLUS

Butanedioic acid. 2,3-dicyano-2,3-bis(4-methylphenyl)-, diethyl ester, (2R,35)-rel- (SCI) (CA INDEX NAME)

Relative stereochemistry.

139257-69-5 CAPLUS Butanedioic acid, 2,3-dicyano-2,3-bis(4-methylphenyl)-, diethyl ester, (Rr.Rr)-, compd. with tetrachloromethane (1:2) (9C1) (CA INDEX NAME)

CM 1

ANSWER 74 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN

ANSWER 75 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN
1991:206840 CAPLUS
114:206840 Synthesis of 5'-[1-(methoxycarbonyl)-2-(p-methoxyphenyl)ethyl)- and
5'-[2-(methoxycarbonyl)-1-(p-methoxyphenyl)ethyl]-2',3',4,4',6'pentamethoxychalcone
Obara, Heitaro: Onodera, Junichi; Tsuchiya, Mitsuhiro; Matsueda, Hiroyuki;
Sato, Shingo; Matsuba, Shigeru
Fac. Eng., Yamagata Univ., Yonezawa, 992, Japan
Bulletin of the Chemical Society of Japan (1991), 64(1), 309-11
CODEN: BCSJA8; ISSN: 0009-2673
Journal
English L4 AN DN TI

English CASREACT 114:206840

Pentamethoxychalcone derivs. (E)-I [R = CO2Me, Rl = p-MeOC6H4CH2 and R = CH2CO2Me, Rl = p-MeOC6H4 (II)] were synthesized from pentamethoxychalcone and 2,3,4,6-(OH) 4CGECOMe, resp. II was completely identical with the methylated derivative of aplycon of safflomin C, a constituent of safflower (Carthamus tinetorius L).

133466-24-7P
RL: SFN (Synthetic preparation); PREP (Preparation) (preparation of)
133466-24-7 CAPLUS
Benzenepropanolic acid, 4-methoxy-a-[2,3,4,6-tetramethoxy-5-[3-(4-methoxyphenyl)-1-oxo-2-propenyl]phenyl]-, methyl ester, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

ANSWER 76 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN
1991:142803 CAPLUS
114:142803 CAPLUS
114:142803 CAPLUS
114:142803 CAPLUS
114:142803 CAPLUS
114:142803 CAPLUS
114:142803 Each of methyl 2,3-diaryl-3-methoxypropanoates by oxidative rearrangement of chalcones using hypervalent iodine reagents in trimethyl orthoformate
Singh, Om V.; Garg, Chandra P.; Kapoor, Ram P.
Dep. Chem., Kurukshetra Univ., Kurukshetra, 132 119, India
Synthesis (1990), (11), 1025-6
CODEN: SYNTBF: ISSN: 0039-7881
Journal
English
CASREACT 114:142803

A diastereoselective synthesis of Me 2,3-diaryl-3-methoxypropanoates I (R = Ph, 4-ClCGH4, Rl = Ph, 4-MeCGH4, 4-MeCGH4) by oxidative rearrangement of RICOCH:CHR with (diacetoxylodo)benzene and hydroxy(tosyloxy)lodobenzene in CHCGH6) 3 is described.

132814-43-89 132814-45-0P
RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of) 132814-43-8 CAPLUS
Benzenepropanoic acid, α-(4-chlorophenyl)-β,4-dimethoxy-, methyl ester, (R\*,R\*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

132814-45-0 CAPLUS Benzenepropanoic acid,  $\alpha$ -(4-chlorophenyl)- $\beta$ -methoxy-4-methyl-, methyl ester, ( $R^*,R^*$ )- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L4 ANSWER 75 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

ANSWER 76 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

ANSWER 77 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN
1991:13787 CAPLUS
114:13787
Electrochemistry of some ethyl o-bromo(dihalophenyl) acetates and
electrochemical synthesis of diastereoisomeric diethyl
2,3-bis(dihalophenyl) succinates
Mattiello, Leonardor De Luca, Carlor Rampazzo, Liliana
Cent. Stud. Elettrochim. Chim. Fis. Interfasi, CNR, Rome, Italy
Journal of the Chemical Society, Perkin Transactions 2: Physical Organic
Chemistry (1972-1999) (1990), (6), 1041-4
CODEN: JCPKEH; ISSN: 0300-9580
JOURNal
English
Et o-bromo-2,4- or -3,4-dihalogenophenylacetates (ABr), where
halogen = F or Cl, are prepared and electrolyzed on reticulated vitreous C
(RVC) in DMF containing EtaNclo4 (0.1 mol dm-3). Potentiostatic reduction

(RVC) in DMF containing Et4NC104 (0.1 mol dm-3). Potentiostatic reduction 1.6 to -1.8 V vs. SCE furnishes the corresponding racemic and meso succinates. Monoesters are also isolated. An excess of racemic isomers is observed for some compds. Voltammetric expts. show practically no difference between the reduction potentials of the isomeric compds. Diastereoisomers can be distinguished by NMR spectroscopy, allowing diastereoisomeric excess to be evaluated before isolation of the single products. A mechanism involving radical intermediates cannot be excluded. On this basis, the diastereoisomeric excess can be explained by assuming different substituents.

129430-56-60 P129430-55-7P 129430-60-0P 129430-61-1P 129430-62-2P 129430-63-3P 129430-64-P 31009-67-1P RL: FORM (Formation, nonpreparative); PREP (Preparation)

(formation of, in electrochem. reduction of bromodihalogenophenyl esters) 129430-63-6 CAPLUS Butanedioic acid. 2,3-bis(2,4-dichlorophenyl)-, diethyl ester, (R\*,5\*)
(PGCI) (CA INDEX NAME)

#### Relative stereochemistry.

129430-59-7 CAPLUS

Butanedioic acid, 2,3-bis(2,4-dichlorophenyl)-, diethyl ester,  $(R^*,R^*)$ -(9CI) (CA INDEX NAME)

Relative stereochemistry.

ANSWER 77 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

129430-63-3 CAPLUS Butanedioic acid, 2,3-bis(3,4-dichlorophenyl)-, diethyl ester, (R\*,R\*)-(SCI) (CA INDEX NAME)

#### Relative stereochemistry.

129430-64-4 CAPLUS Butamedicic acid, 2,3-bis(3,4-difluorophenyl)-, diethyl ester, (R\*,5\*)-(9C1) (CA INDEX NAME)

#### Relative stereochemistry.

131009-67-1 CAPLUS
Butanedioic acid, 2,3-bis(3,4-difluorophenyl)-, diethyl ester, (R\*,R\*)-(9CI) (CA INDEX NAME)

Relative stereochemistry.

L4 ANSWER 77 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

129430-60-0 CAPLUS
Butanedioic acid, 2,3-bis(2,4-difluorophenyl)-, diethyl ester, (R\*,S\*)-(9CI) (CA INDEX NAME)

Relative stereochemistry.

129430-61-1 CAPLUS Butanedioic acid, 2,3-bis(2,4-difluorophenyl)-, diethyl ester, (R\*,R\*)-(9CI) (CA INDEX NAME)

#### Relative stereochemistry.

129430-62-2 CAPLUS

Butanedioic acid, 2,3-bis(3,4-dichlorophenyl)-, diethyl ester, (R\*,S\*)-(9CI) (CA INDEX NAME).

Relative stereochemistry.

ANSWER 77 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

ANSWER 78 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1990:198049 CAPLUS 112:198049
Preparation of some chromans substituted at the 3- or 4-position by an aryl or benzyl group by the rhodium-catalyzed intramolecular nucleophilic substitution of the corresponding 3-(2-fluorophenyl)propan-1-ols Houghton, Roy P.: Shervington, Leroy A. Coll. Cardiff, Univ. Wales, Cardiff, CPI 3TB, UK JOURNAI of Chemical Research, Synopses (1989), (8), 239 CODEN: JRPSDC: ISSN: 0308-2342 JOURNAI English CASREACT 112:198049

[Rh(n5-CSEtMe4) (n6-C6H6)][PF6]2 catalyzed the formation of chromans (I; R = H, CH2OH, Ph, 2-PCGH4, CH2Ph; RI = Ph, 4-O2NCGH4, 4-MeCCGH4, CH2OH, H) from 2-PCGH4(CHCCHH2ICH) in MeNO2-Me2CO. 126348-14-9P
RI: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

RE: NCT (Reactain, 727 (77) (Reactain of reagent)
(preparation and reduction of)
126348-14-9 CAPLUS
Butanedioic acid, 2,3-bis(2-fluorophenyl)-, dimethyl ester (9CI) (CA

ANSWER 80 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1988:473717 CAPLUS 109:73717

109:73717
Stereoselective synthesis of the dihydrobenzo[b]furan segments of the ephedradine alkaloids
Baker, Raymond: Cooke, Nigel G.; Humphrey, Guy R.; Wright, Stanley H. B.; Hirshfield, Jordan
Dep. Chem., Univ. Southampton, Southampton, SO9 5NH, UK
Journal of the Chemical Society, Chemical Communications (1987), (14), 1102-4

CODEN: JCCCAT; ISSN: 0022-4936

Journal English CASREACT 109:73717

Dihydrobenzofuran derivs. I (R, R1 = H, MeO; R2 = H, Me) were prepared via Levis-catalyzed cyclization of phenol substituted β-hydroxy esters II as key step; the use of chiral oxazolidinones in the aldol reaction has formed the basis of enantiospecific syntheses of III (R3 = CO2Me, CH2OH). 115439-21-pp 115439-22-0p 115439-23-1p 115439-23-1p 115439-27-SP 115439-28-6P 115439-27-P 115439-28-6P 115439-27-P 115439-28-6P 115439-27-P

115465-67-3P
RL: RCT (Reactant): SPN (Synthetic preparation); PREP (Preparation): RACT (Reactant or reagent)
(preparation and intramol. cyclization of, benzofuran derivative from)
115439-21-9 CAPLUS
Benzenepropanoic acid, a-{5-{dimethoxymethyl}-2-{phenylnethoxymethyl}-p,4-dihydroxy-, methyl ester, (R\*,R\*)- (9CI)
(CA INDEX NAME)

Relative stereochemistry.

ANSWER 79 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1990:178248 CAPLUS 112:178248 112:178248 CAPLUS 1200 ACS OF TAXABLE PROPERTY OF TAXABLE

III

AB (Z)-2-H02CC6H4C(C02R):CHC6H4Cl-3 (I: R = Me)(II) was heated with aqueous NaOH

to give the dibasic acid I (R = H), which was converted to the cyclic anhydrides (Z)-III (IV) and (E)-III. IV was cyclized with AlCl3 to give indenyl acid V. Bromination, lactonization and cyclization of II was studied. The reaction of II and IV with primary amines, hydroxylamine, hydrazine, Ph hydrazine and p-nitrophenylhydrazine were also investigated. 126558-65-4P

126558-65-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
126558-65-4 CAPLUS
Benzenepropanoic acid, α,β-dibromo-α-(2-carboxyphenyl)-3-chloro-, monomethyl ester (9CI) (CA INDEX NAME)

ANSWER 80 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

115439-22-0 CAPLUS

115439-22-0 CAPLOS Benzenepropanoic acid, a-{5-(dimethoxymethyl)-2-(phenylmethoxy)phenyl]-B,4-dihydroxy-3-methoxy-, methyl ester, (R\*,5\*)- (9CI) (CA INDEX NAME).

Relative stereochemistry.

115439-23-1 CAPLUS
Benzenepropanoic acid, a-[5-(dimethoxymethyl)-2-(phenylmethoxy)phenyl)-B,4-dihydroxy-3-methoxy-, methyl ester,(R\*,R\*)-(9CI) (CA INDEX NAME)

Relative stereochemistry.

115439-24-2 CAPLUS
Benzenepropanoic acid. a-{5-(dimethoxymethyl)-2-

ANSWER 80 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) (phenylmethoxy) phenyl]- $\beta$ -hydroxy-3,4-dimethoxy-, methyl ester, (R\*,S\*)- (9CI) (CA INDEX NAME)

115439-25-3 CAPLUS Benzenepropanoic acid,  $\alpha$ -[5-(dimethoxymethyl)-2-(phenylmethoxy)phenyl]- $\beta$ -hydroxy-3,4-dimethoxy-, methyl ester, (R\*,R\*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

115439-26-4 CAPLUS Benzenepropanoic acid,  $\alpha$ -[5-(dimethoxymethyl)-3-methoxy-2-(phenylmethoxy)phenyl)- $\beta$ ,4-dihydroxy-, methyl ester, ( $R^*$ , $S^*$ )- (9CI) (CA INDEX NAME)

Relative stereochemistry.

ANSWER 80 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) (phenylmethoxy)phenyl]-B-hydroxy-4-methoxy-, methyl ester, (R\*,R\*)-(9CI) (CA INDEX NAME)

Relative stereochemistry.

115465-67-3 CAPLUS Benzenepropanoic acid,  $\alpha$ -{5-(dimethoxymethyl)-2-(phenylmethoxy)phenyl}- $\beta$ ,4-dihydroxy-, methyl ester, (R\*,S\*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

ANSWER 80 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

115439-27-5 CAPLUS
Benzenepropanoic acid, α-[5-(dimethoxymethyl)-3-methoxy-2(phenylmethoxy)phenyl]-β,4-dihydroxy-, methyl ester, (R\*,R\*)- (9CI)
(CA INDEX NAME)

Relative stereochemistry

115439-28-6 CAPLUS
Benzenepropanoic acid, a-[5-(dimethoxymethyl)-2-(phenylmethoxy)phenyl]-B-hydroxy-4-methoxy-, methyl ester, (R\*,S\*)-(9CI) (CA INDEX NAME)

Relative stereochemistry.

115439-29-7 CAPLUS Benzenepropanoic acid,  $\alpha$ -[5-(dimethoxymethy1)-2-

L4 AN DN TI

AU CS SO

ANSWER 81 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN
1988:131218 CAPLUS
108:131218 CAPL

electrolyzing di-Me bromomalonate and related compass. In absolute containing
0.1M Ba(Cl04)2 as electrolyte on nickel cathode at controlled potential.
A suitable mechanism involving the formation of malonate carbanion intermediate is suggested.

IT 34404-72-3 34404-73-4P
RL: SPN (Synthetic preparation): PREP (Preparation)
(preparation of)
RN 34404-72-3 CAPLUS
CN 1,1,2,2-Ethanetetracarboxylic acid, 1,2-bis(4-methylphenyl)-, tetramethylester (9CI) (CA INDEX NAME)

34404-73-4 CAPLUS
1,1,2,2-Ethanetetracarboxylic acid, 1,2-bis(4-chlorophenyl)-, tetramethyl ester (9CI) (CA INDEX NAME)

L4 AN DN TI

ANSWER 82 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN
1988:131203 CAPLUS
108:131203 CAPLUS
108:131203 captus
108:131203 capt

Electrochem. reduction of 4-RC6H4CHBCO2Et (I: R = Br, Cl, F) gave the (i)-and meso-isomers of 4-RC6H4CH(CO2Et)CH(CO2Et)C6H4R-4, epoxides II, and 4-RC6H4CHC2C02Et. The (i)- and meso-isomers were identified by NHC 4-RCDHKCH/COZET. The (f)- and meso-isomers were identified by NMR spectroscopy.
113387-87-4P 113387-88-5P 113387-90-9P 113387-91-10P 113387-91-2P 113387-94-3P RL: FORM (Formation, nonpreparative); PREP (Preparation) (formation of, in electrochem. reduction of bromo(halophenyl)acetate) 113387-87-4 CAPLUS

Butanedioic acid, 2,3-bis(4-fluorophenyl)-, diethyl ester, (R\*,S\*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

113387-88-5 CAPLUS Butanedioic acid, 2,3-bis(4-fluorophenyl)-, diethyl ester, (R\*,R\*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

ANSWER 82 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN

113387-94-3 CAPLUS Butanedioic acid, 2,3-bis(4-bromophenyl)-, diethyl ester, (R\*,R\*)- (9CI) (CA INDEX NAME)

Relative stereochemistry

ANSWER 82 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

113387-90-9 CAPLUS

Butanedioic acid, 2,3-bis(4-chlorophenyl)-, diethyl ester, (R\*,5\*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

113387-91-0 CAPLUS Butanedioic acid, 2,3-bis(4-chlorophenyl)-, diethyl ester, (R\*,R\*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

113387-93-2 CAPLUS Butanedioic acid, 2,3-bis(4-bromophenyl)-, diethyl ester, (R\*,S\*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

ANSWER 83 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN
1987:635925 CAPLUS
107:235925
The different recombinations of diphenylmethyl radicals, Ph2C(-)R
(R = CMe3 CN, COZR', COR')
Neumann, W. P., stapel, R.
Univ. Dortmund, Dortmund, D-6600/50, Fed. Rep. Ger.
NATO ASI Series C: Mathematical and Physical Sciences (1986),
189(Substituent Eff. Radical Chem.), 219-22
CODEN: NSCSW#, ISSN: 0258-2023
Journal
English
ESR data for radicals R21CR= (R1 = Ph, p-anisyl, p-tert-butylphenyl; R
- Me3C, SiMe3, COZMe, COZET, COZCHZPh, CHO, COPh, etc.) and dissociation
enthalpies of their dimers are measured.
104505-55-7
RAFUES
(dissociation enthalpy of)
104505-55-7 CAPLUS
Butanedioic acid, tetrakis[4-(1,1-dimethylethyl)phenyl]-, dimethyl ester
(9CI) (CA INDEX NAME)

ANSWER 84 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1987:196146 CAPLUS 106:196146 Estrogenic affinity labels: synthesis, irreversible receptor binding, and bioactivity of aziridine-substituted hexestrol derivatives 2ablocki, Jeffery A.; Katzenellenbogen, John A.; Carlson, Kathryn E.; Norman, M. J.; Katzenellenbogen, Benita S. Dep. Chem., Univ. Illinois, Urbana, IL, 61801, USA Journal of Medicinal Chemistry (1987), 30(5), 829-38 CODEN: JMCMAR; ISSN: 0022-2623 Journal English CASREACT 106:196146

Aziridine derivs. (e.g., I) of the potent nonsteroidal estrogen hexestrol [(3R\*,4S\*)-3,4-bis(4-hydroxyphenyl)hexane] were prepared as affinity labels for the estrogen receptor that are estrogen agonists, rather than antagonists. Thus, the mesylate II was treated with ethylenimine to give 50% 1. In these compds. the hexestrol ligand and the aziridine are linked by a carbonyl group (ketone or estee), a thio ether, or a methylene chain. The apparent competitive binding affinity of these derivs. for the estrogen receptor ranges from 1.8% to 25% that of estradiol, and most of them bind in a time-dependent, irreversible manner with the receptor, although the rate and efficiency of this binding vary widely, often with relatively small changes in structure. This is consistent with the irreversible attachment requiring a precise alignment of activating and reacting residues in the binding site of the receptor. The estrogenic and antiestrogenic activity of these aziridine derivs. was investigated in MCF-7 human breast cancer cells. Most of the compds. are agonists, with one being an antagonist. I has the most ideal behavior of the estrogenic affinity labeling agents prepared It is an agonist, and it binds to receptor irreversibly, efficiently, and quite rapidly. 107036-27-1P 107036-28-2P RL: RCT (Reactant): SPN (Synthetic preparation): PREP (Preparation): RACT (Beactant): S

Relative stereochemistry.

ANSWER 84 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Contine Benzenepropanoic acid,  $\beta$ -ethyl-4-hydroxy- $\alpha$ -(4-hydroxyphenyl)-, 2-(1-aziridinyl)ethyl ester, (R\*,S\*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

ANSWER 84 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

107036-28-2 CAPLUS Benzenepropanoic acid,  $\beta$ -ethyl-4-hydroxy- $\alpha$ -(4-hydroxyphenyl)-, 2-iodoethyl ester, (R\*,5\*)- (9C1) (CA INDEX NAME)

Relative stereochemistry.

107036-09-9P 107036-10-2P

RL: SPN (Synthetic preparation): PREP (Preparation)
(preparation and estrogen receptor binding affinity and agonist activity

107036-09-9 CAPLUS

Benzenepropanoic acid, β-ethyl-4-hydroxy-α-(4-hydroxyphenyl)-, 3-(1-aziridinyl)propyl ester, (R\*,5\*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

107036-10-2 CAPLUS

ANSWER 85 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1987:66855 CAPLUS 106:66855

106:66855
Sterically hindered free radicals. XVI. The existence of tetraphenylsuccinic acid and its esters, and the structur of the diarylmethyl radicals RZC-X (X ~ COZRI, CN, CORI) Neumann, Wilhelm P.; Stapel, Ralf Univ. Dortmund, Dortmund, D-4600/50, Fed. Rep. Ger. Chemische Berichte (1986), 119(11), 3422-31
CODEN: CHBEAN; ISSN: 0009-2940
Journal cture of the dimers

CS SO

CASREACT 106: 66855

The coupling of Ph2CBrCO2Et in refluxing C6H6 containing Cu powder followed

rearrangement and deesterification gave 1,4-{Ph2C(CO2H)}CGH4. Also prepared were MeO2C(CGH4CMe3-4)2C(CGH4CMe3-4)2CCQMe, Ph2C:CGCPh2COR (R = H, Me, Ph), and di-Me 9,9'-bifluorene-9,9'-dicarboxylate. The ESR of R22C=R3 (R2 = Ph, 4-Me3CCGH4: R3 = CO2Me, cyano, CHO, Ac, Bz) and heats of dissociation of the radical dimers were determined 104505-55-7P

IT

ANSWER 86 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1986:206811 CAPLUS 104:206811 104:206811
Reactions with stable phenoxyl radicals
De Jonge, Cornelis R. H. I.
Corp. Res. Dep., Akor Res., Arnhem, Neth.
Lichigs Annalen der Chemie (1986), (2), 299-304
CODEN: LACHDL: ISSN: 0170-2041
JOurnal
English English CASREACT 104:206811

Phenoxyl radical I was generated and underwent H abstraction reactions with Me, methylene, and methine compds. to form ethers. Triply activated compds. Ph2CHCN and p-MeCGH4CH(CN)CO2Me underwent C-C dimerization on treatment with I. 31249-0.3-2ĪΤ

31249-03-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
31249-03-3 CAPUS
Butanedioic acid, 2,3-dicyano-2,3-bis(4-methylphenyl)-, dimethyl ester
(9CI) (CA INDEX NAME)

ANSWER 87 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

ANSWER 87 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN
1986:148061 CAPLUS
104:148061 CAPLUS
104:148061 CAPLUS
104:148061 CAPLUS
104:148061 CAPLUS
104:148061 CAPLUS
105:148061 CAPLUS
105:148061 CAPLUS
106:148061 CAPLUS
107:148061 CAPL AU CS SO

English CASREACT 104:148061

11 CO2Et TIT

The anodic coupling reactions of 4-benzylisochromanone I and 4-benzyl-1,2,3,4-tetrahydroisoquinolines II (R = Me, RI = H; R= Me, CO2Et, CHO, RI = OMe) were studied and compared. In neutral media II gave products of coupling to C-1 and/or N-2, depending on the ring substituents. In acid solution, II gave isoaporphines, whereas the 1-benzyl analogs couple at C-8 to give morphinedienones. The different regionselectivities are due to inductive effects in the protonated bases. I also couples at C-8 but the resulting, intermediate is unstable and reacts further with nucleophiles to give 24% 2,5-(OHC) (MeO/CHGCHGHOWHO-2) and 6.3% phenathrene III. 98748-60-8P
RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of, by regionselective anodic oxidation-ring cleavage of isochromanones) 98748-60-8 CARLUS Benzenepropanoic acid, a-(2-formyl-5-methoxyphenyl)-3-methoxy-,

Benzenepropanoic acid,  $\alpha$ -(2-formyl-5-methoxyphenyl)-3-methoxy-, methyl ester (CA INDEX NAME)

L4 ANSWER 88 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1985:45575 CAPLUS
DN 102:45575
CAPLUS
COREF 102:7157a,7160a
TI Synthetic studies in polycyclic systems: part IX - synthesis of methoxy derivatives of IHH-benzo[a]fluorenes and 1H-naphtho[2,1-a]fluorenes
AU Rao, Alaka: Lala, Sunandan: Rao, R. R.
CD Dep. Chem., Visva-Bharati Univ., Santiniketan, 731 235, India
SO Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry [1984], 23B(7), 603-10
CODEN: 1JSBDB: ISSN: 0376-4699
DT Journal
LA English
CS CASREACT 102:45575

Michael reaction of RCH:CHCO2Et [R = CGH40Me-2, -3, -3, CGH3COMe)2-3, 4] with R1CH2CO2Et [R1 = Ph, 2-naphthy1] gave 75-86t Eto2CCHR1CHRCH2CO2Et, which was hydrolyzed to give MOZCCHR1CHRCH2CO2H. The diacids were cyclized with SnCl4 to give 54-66t tetralone derivs. 1 (R2 = R3 = H, CH:CHCHCH; X = 0) which were reduced with Zn or HZNN12 to give 54-67, 59-66t 1 (X = H2) resp. The last were methylated, dehydrogenated, and saponified to give naphthalene- and phenanthrenecatboxylic acids II (same R's), which were cyclized using H2SO4, AlCl3, or SnCl4 to give 18-38, 29-42, 52-74t fluorenone derivs. III (R4 = R6 = OMe, R3 = H; R4 = OMe, R5 = R6 = H; R4 = R6 = H, R5 = OMe; R4 = R5 = H, R6 = OMe, X6 = 0), resp. The ketones were reduced with HZNNH2 to give 54-67t title compds. III (same R's, X1 = H2). 94146-62-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and saponification of) 94146-62-0 CAPLUS
Pentanedioic acid, 2-{2-(ethoxycarbonyl)phenyl]-3-(2-methoxyphenyl)-, diethyl ester (9CI) (CA INDEX NAME)

IT 94146-63-1P 94146-64-2P 94146-65-3P
RL: RCT (Reactant): SPN (Synthetic preparation): PREP (Preparation): RACT (Reactant or reagent)
(preparation, hydrolysis, and Dieckmann cyclization of)
RN 94146-63-1 CAPLUS
CN Pentamedioic acid, 2-[2-(ethoxycarbonyl)phenyl]-3-(3-methoxyphenyl)-, diethyl ester (9CI) (CA INDEX NAME)

94146-64-2 CAPLUS
Pentanedioic acid, 2-[2-(ethoxycarbonyl)phenyl]-3-(4-methoxyphenyl)-, diethyl ester (9CI) (CA INDEX NAME)

94146-65-3 CAPLUS
Pentanedioic acid, 3-(3,4-dimethoxyphenyl)-2-[2-(ethoxycarbonyl)phenyl]-,
diethyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 89 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1984:120280 CAPLUS
DN 100:120280
CORET 100:120280
TELECTROCHEMICAL Synthesis of 5,6,11,12-tetrahydro-5,6,11,12-tetrakis(ethoxycarbonyl)dibenzo[a,e]cyclooctene
AU De Luca, Carlor Inesi, Achiller Rampasso, Liliana
CS Cent. Stud. Elettrochim. Chim. Fis. Interfasi, CNN Roma, Rome, Italy
Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1972-1999) (1981), (12), 1821-5
CDDEN: JCPKBH: ISSN: 0300-9580
DT Journal
LA English
G1

DT LA GI

CO2Et CO2Et COZEt

Electrochem. reduction of 1,2-(Et02CCHBr)2CGH4 (I) in DMF at a vitreous C electrode gave 15% 1,2-(Et02CCH2)2CGH4, 16% title compound (II), 16% [o-Et02CCH2CGH4CH(COZET)]2 and 20% polymer as the major products. Only apprx.N1 of benzocyclobutene III was formed. The intermediate formation of c,a'-bis(ethoxycarbonyl)-o-quinodimethane, whose behavior resembles that of a biradical, through the 2 electron electrochem. reductive elimination of the Br- ions from I, is the key step in this reaction.

B9215-22-5P 89215-23-6P 89215-24-7P
RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

B9215-22-5 CAPIUS
Butanedioic acid, 2,3-bis[2-(2-ethoxy-2-oxoethyl)phenyl]-, diethyl ester, (R\*,5\*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

 $\label{eq:continuous} \begin{array}{ll} \text{89215-23-6} & \text{CAPLUS} \\ \text{Butanedioic acid, 2,3-bis[2-{2-ethoxy-2-oxoethyl}]phenyl}-, \ \text{diethyl ester,} \\ \text{(R*,R*)- (9CI)} & \text{(CA INDEX NAME)} \end{array}$ 

ANSWER 88 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN

L4 ANSWER 89 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN Relative stereochemistry. (Continued)

89215-24-7 CAPLUS 1,2-Benzenedipropanoic acid,  $\beta,\beta'$ -bis(ethoxycarbonyl)- $\alpha,\alpha'$ -bis[-2(2-ethoxy-2-oxoethyl)phenyl]-, diethyl ester,  $(\alpha R^*,\alpha'R^*,\beta R^*,\beta'R^*)$ - (9CI) (CA INDEX NAME)

ANSWER 90 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1983:453253 CAPLUS
DN 99:53253
OREF 99:8309a
TI The sensitized photooxidation of methyl (E)-ferulate
AU Kuo, Yueh Hsiung: Kuo, Pao Chu: Lin, Sheng Tsair
CS Dep. Chem., Natl. Taiwan Univ., Taipei, Taiwan
Froceedings of the National Science Council, Republic of China, Part B:
Basic Science (1983), 7(1), 28-34
CODEN: PCRCO3; ISSN: 0253-6070
DT Journal

Journal English

The title reaction gave 4 products, Me (2)-ferulate, vanillin, I, and II. Product structures were elucidated by chemical derivs. 86069-39-86069-40-1P

ΙT

86069-39-8P 86069-40-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
86069-39-8 CAPLUS
Benzenepropanoic acid, 4-hydroxy-a-{2-hydroxy-3-methoxy-5-{3-methoxy-3-oxopropyl)phenyl}-3-methoxy-, methyl ester (CA INDEX NAME)

86069-40-1 CAPLUS

Benzenepropanoic acid, 4-{acetyloxy}-a-[2-(acetyloxy)-3-methoxy-5-(3-methoxy-3-oxopropyl)phenyl]-3-methoxy-, methyl ester (CA INDEX NAME)

ANSWER 91 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN
1983:218134
98:218134
99:33153a,33156a
Fluorescent chelates and labeled specific binding reagents prepared from them
Hinshaw, Jerald Clyder Toner, John Luker Reynolds, George Arthur
Eastman Kodak Co., USA
Eur. Pat. Appl., 50 pp.
CODEN: EPXXDW
Patent
English
CNT 2

DT LA

100	English				
FAN.	CNT 2				
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 68875	A2	19830105	EP 1982-303380	19820628
	EP 68875	A3	19830504		
	EP 68875	B1	19871223		
	R: DE, FR, GB				
	CA 1205028	A1	19860527	CA 1982-405050	19820611
	JP 58009783	A	19830118	JP 1982-112653	19820701
	JP 06014042	В	19940223		
	US 4637988	λ	19870120	US 1986-825693	19860203
	US 4670572	A	19870602	US 1986-825009	19860203
	US 4801722	Α	19890131	US 1987-7024	19870127
	US 4794191	A	19881227	US 1988-151847	19880203
	US 4859777	A	19890822	US 1988-285163	19881216
PRAI	US 1981-279398	A	19810701		
	US 1986-825693	A3	19860203		
	US 1987-7024	A3	19870127		
	US 1987-40385	A3	19870420		

Disprior No. 1 19870420

CASREAT 98:218134: MARPAT 98:218134

Stable fluorescent chelates are manufactured comprising a complex of a lanthanide metal and a chelating agent that includes a mostey that is a triplet energy greater than that of the lanthanide metal and at least 2 heteroatom-containing groups that form coordinate complexes with lanthanide metals and a 3rd heteroatom-containing group or heteroatom in or appended to the triplet sensitizer. Thus, a benzoylhydroxybis (N. M-bis (carboxylate) minomethyl) commanin-Eu chelate was used with an anal. test element containing oxidumin and normal rabbit serum and the fluorescence signal was a function of the concentration of the Euchelate. The chelate is useful to label a variety of physiol. active materials by binding then to the complex by adsorption or by covalent bonding. The materials are especially useful in specific binding assay cods.

bonding. The materials are especially useful in specific binding assay methods.

IT 85929-38-0P
RL: RCT (Reactant): SPN (Synthetic preparation): PREP (Preparation): RACT (Reactant or reagent)
(preparation and hydrolysis of)
RN 85925-38-0 CAPUSIS
CN Benzenepropanoic acid, a-[3-[4-(acetyloxy)-3,5-bis[[bis[2-(1,1-dimethylehoxy)-2-oxoethyl]maino]methyl]benzoyl]phenyl]-4-(4-hydroxy-3,5-diiodophenoxy)-3,5-diiodo-, methyl ester (CA INDEX NAME)

ANSWER 90 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN

ANSWER 91 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN

PAGE 1-A

PAGE 1-B

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85916-19-4P
RL: PREP (Preparation)
(preparation of)
85916-19-4 CAPLUS
Benzenepropanoic acid,  $\alpha$ -[3-[3,5-bis[[bis(carboxymethyl)amino]methyl]
1-4-hydroxybenzoyl]phenyl]-4-(4-hydroxy-3,5-diiodophenoxy)-3,5-diiodo-,  $\alpha$ -methyl ester (9CI) (CA INDEX NAME)

ANSWER 92 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN
1981:8867 CAPLUS
98:13847a,13550a
Thermal, photochemical, and acid-catalyzed rearrangements of the spiro
diner of a,a'-bis(methoxycarbonyl)-o-quinodimethane. X-ray
crystal structure of trans,trans-tetrakis(methoxycarbonyl)dibenzo[a,e]cycl
ooctene
Jones, David W.; McDonald, Walter S.
Dep. Org. Chem., Univ. Leeds, Leeds, Ls2 9JT, UK
Journal of the Chemical Society, Perkin Transactions 1: Organic and
Bio-Organic Chemistry (1972-1999) (1982), (9), 2257-63
CODEN: JCPRB4: ISSN: 0300-922X
JOURNAL
English

The stereochem. of the title spiro-dimer I (R = R2 = CO2Me, R1 = R3 =  $\{II\}$  was determined by comparison of its properties with those of the

ANSWER 92 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of) 84198-36-7 CAPLUS (Continued)

1,2-Benzendeiacetic acid, a-[2-methoxy-1-[2-(2-methoxy-2-oxoethyl)phenyl]-2-oxoethyl]-a'-phenyl-, dimethyl ester (9CI) (CA INDEX NAME)

84198-40-3 CAPLUS 1,2-Benzenediacetic acid,  $\alpha-[2-methoxy-1-[2-(2-methoxy-2-oxoethyl)phenyl]-2-oxoethyl]-, dimethyl ester, <math>(R^*,R^*)-$  (9CI) (CA INDEX

Relative stereochemistry.

ANSWER 92 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continue. 1, 2-Benzenediacetic acid,  $\alpha$ -[2-methoxy-1-[2-(2-methoxy-2-cxoethyl)phenyl]-2-oxoethyl]- $\alpha$ -"[[(4-methylphenyl)sulfonyl]oxy]-, dimethyl ester, [ $\alpha$ R\*(R\*), $\alpha$ \*S\*]- (9C1) (CA INDEX NAME) (Continued)

84275-76-3 CAPLUS
1,2-Benzenediacetic acid, a-[2-methoxy-1-[2-{2-methoxy-2oxoethyl]-phenyl]-2-oxoethyl]-a'-[[(4-methylphenyl)sulfonyl)oxy]-,
dimethyl ester, [aR\*(R\*),a'R\*]- (9CI) (CA INDEX NAME)

84198-36-7P 84198-40-3P

ANSWER 93 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1982:556714 CAPLUS 97:156714 97:156714 97:156714 97:25985a, 25988a (2R\*,35\*)-1-[1251]Iodo-2,3-bis(4-hydroxyphenyl)pentane ([1251]iodonorhexestrol), and (2R\*,35\*)-1-[77Br]bromo-2,3-bis(4-hydroxyphenyl)pentane ([77Br]bromonchexestrol), two \( \gamma\)-emitting estrogens that show receptor-mediated uptake by target tissues in vivo Landvatter, Scott W.: Katzenellenbogen, John A.: McElvany, Karen D.: Welch, Michael J.
Sch. Chem. Sci., Univ. Illinois, Urbana, IL, 61801, USA Journal of Medicinal Chemistry (1982), 25(11), 1307-12 CODEN: JMCMAR: ISSN: 0022-2623 Journal English ΑU

CS SO

Two y-emitting estrogen analogs, (2R,3S)-1-[1251]iodo-2,3-bis(4-hydroxyphenyl)pentane (I) [83181-42-4] and (2R,3S)-1-[77Br]bromo-2,3-bis(4-dydroxyphenyl)pentane (II) [83181-42-5] were prepared by halide ion displacement on a labile trifluoromethanesulfonate derivative of a suitably protected precursor, followed by mild acid deprotection. Although halide displacement on a more stable tristrifluoromethanesulfonate derivative was successful, the basic conditions required for deprotection of this precursor resulted in destruction of the products by a base-induced spiroelimination reaction. In immature female rats, both of these halonorhexestrols demonstrated preferential uptake by the uterus that could be selectively blocked by coadministration of a large dose of unlabeled estradiol. In a double label comparison with 16e-[1251]iodo-17B-estradiol, the uterine uptake of II was notably less selective. Stability studies in vitro and in vivo indicated that both I and II are quite labile, and this lability compromises the selectivity of their uptake by estrogen target tissues in vivo. p-Hydroxyphenethyl halides are known to be unusually prone to a base-catalyzed solvolysis, via cyclization of the phenolate to a spirocyclohexadienone intermediate. This unusual solvolytic mechanism may contribute to the lability of these halonorhexestrols in vivo. 83213-76-7 CAPLUS
Benzenepropanoic acid, p-ethyl-4-hydroxy-a-(4-hydroxyphenyl)-, methyl ester, (R,\*5)- (9CI) (CA INDEX NAME)

Benzenepropanoic acid, B-ethyl-4-hydroxy-a-(4-hydroxyphenyl)-, methyl ester, (R\*,5\*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

ANSWER 93 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

ANSWER 95 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1981:615317 CAPLUS 95:215317 95:35821a,35824a OREF TI Stereochemical considerations in the binding of nonsterd the estrogen receptor Landwatter, Scott W.: Katzenellenbogen, John A. Sch. Chem. Sci., Univ. Illinois, Urbana, IL, 61801, USA Molecular Pharmacology (1981), 20(1), 43-51 CODEN: MOPMA3: ISSN: 0026-895X Journal English Stereochemical considerations in the binding of nonsteroidal estrogens to

Derivs. of nonsteroidal estrogens, such as hexestrol, can interact with the estrogen receptor in 4 possible binding modes, 2 per enantiomer. Several side chain-functionalized hexestrol and norhexestrol derivs, have been synthesized and resolved into pure enantiomers. Binding studies with lamb uterine estrogen receptor have indicated that there is no appreciable difference in binding. The (-) (2R, 35) -pentyl ester (1) [ 79568-12-0] binds to receptor with twice the affinity of racemic material and 14 times the affinity of the (+)-(2R, 3R)-antipode [79923-77-0]. It is concluded that the norhexestrols prefer l of the 4 possible binding modes, whereas the hexestrols can adopt 2 of the 4 modes equally. Furthermore, comparisons between the binding affinities of corresponding hexestrol and norhexestrol derivs. suggest that the source of chiral recognition is a specific interaction between the carbonyl group in the 2R, 35 enantiomer of the norhexestrol derivs. that elevates affinity, this interaction not being attainable in the other enantiomer and in the derivs. in the hexestrol series.

79568-12-07 79618-13-67 79618-14-7P
79645-19-58 83213-76-7P
RL: SPN (Synthetic preparation), PREF (Preparation) (preparation and estrogen receptor binding of)
79568-12-O CAPLUS
Benzenepropanoic acid, β-ethyl-4-hydroxy-a-(4-hydroxyphenyl)-, nearly learn. [R-67, Syll-(67)] (CA INDEX NAME)

Penzenepropanoic acid, β-ethyl-4-hydroxy-α-(4-hydroxyphemyl)-, pentyl ester, [R-(R\*,S\*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 94 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1982:527210 CAPLUS
DN 97:127210
OREF 97:21105a, 21108a

II Uncatalyzed insertion reaction of isocyanides into a carbon-sulfur bond
AN Morel, G.r Marchand, E.r Nguyen Thi, K. H.r Foucaud, A.
CS Groupe Physiochim. Struct., Univ. Rénnes, Rennes, 35042, Fr.
SO Tetrahedron Letters (1982), 23(19), 2023-6
COODE: TELEAY: ISSN: 0040-4039

DT Journal
La English
OS CASREACT 97:127210
AB RNC (I; R = Me3C, tert-octyl) with RIC(CN) (SR2)COZHe [II; R1 = PhZC(CN), R R2 = Me, Ph, PhCH2: R1 = 5-cyanofluoren-5-yl. (PhCH2)ZC(CN), PhCMe(CN), PhCEC(CN), R2 = Me] at room temperature for 17-114 h gave 36-844
RN:C(SR2)CR1(CN)COZMe (III). III (R2 ≠ Ph) are unstable and
restrange at room temperature to give E- and Z-RN(COZMe)C(SR2):CR1(CN) (E-Z-IV) in 6-82% yield. I with II [Rl = p-R3C6H4 (R3 = Cl, Me, MeO, NO2), PhCH2, R2 = Me; Rl = p-MeC6H4, R2 = PhCH2; Rl = R2 = Ph] in reluxing MeCN gave the corresponding E- and Z-IV in 19-94% yield.
31249-03-3. PRL: SFN (Synthetic preparation); PREP (Preparation) (preparation of) 31249-03-3 CAPLUS
Butanediota caid, 2,3-dicyano-2,3-bis(4-methylphenyl)-, dimethyl ester (9CI) (CA INDEX NAME)

ANSWER 95 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

79618-13-6 CAPLUS Benzenepropanoic acid,  $\beta$ -ethyl-4-hydroxy- $\alpha$ -(4-hydroxyphenyl)-, methyl ester, [S-(R\*,S\*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

79618-14-7 CAPLUS Benzenepropanoic acid,  $\beta$ -ethyl-4-hydroxy- $\alpha$ -(4-hydroxyphenyl)-, methyl ester, [R-(R\*,S\*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

79645-19-5 CAPLUS Benzenepropanoic acid,  $\beta$ -ethyl-4-hydroxy- $\alpha$ -(4-hydroxyphenyl)-, pentyl ester, (R\*,S\*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 83213-76-7 CAPLUS

ANSWER 95 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) Benzenepropanoic acid,  $\beta$ -ethyl-4-hydroxy- $\alpha$ -(4-hydroxyphenyl)-, methyl ester, (R\*,S\*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

AN	1981:30582 CAPLUS	5				
DN	94:30582					
OREF	94:5043a,5046a					
IT	Homophthalimides of	carrying	amino subst	ituents in the 2-positi	on	
IN	Kutter, Eberhard;	Austel,	Volkhard: E	berlein, Wolfgang: Heid	er, Joachim:	
	Kobinger, Walter;	Lillie,	Christian;	Kadatz, Rudolf		
PA	Thomae, Dr. Karl,	G.m.b.H	, Fed. Rep.	Ger.		
so	Can., 74 pp.					
	CODEN: CAXXA4					
DT	Patent					
LA	English					
FAN.	CNT 3					
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
PI	CA 1076116	A1	19800422	CA 1976-258095	19760729	
	DE 2533986	A1	19770217	DE 1975-2533986	19750730	
	DE 2533986	B2	19790906			
	DE 2533986	C3	19800522			
	DE 2622690	A1	19771208	DE 1976-2622690	19760521	
PRAI	DE 1975-2533986	A	19750730			
	DE 1976-2622690	A	19760521			

L4 ANSWER 97 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN

Amines I (X, X1 = C2-4 alkylene, optionally substituted by Me or Ph; R, R1, R7, R8 = H, F, C1, Br, OH, NHZ, NO2, NHAc, alkyl, alkoxy, alkylthio; R2, R3, R5, R6 = H, alkyl, phenylalkyl, methoxyphenylalkyl; R2R3, R5,R6 = Alkylene; R4 = H, alkyl, phenylalkyl) were prepared Thus, 4,4-dimethyl-1,3-isochromandione was treated with MeNI(CH2)NH2[2 to give 65% II. II had an antiarrhythmic ED50 5.5 mg/alm measured on the refractory period of isolated guinea pig left auricle. 76065-15-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(saponification of)
76065-15-1 CAPIUS
Benzenepropanoic acid, 4-methoxy-q-[2-(methoxycarbonyl)phenyl]-e-methyl-, methyl ester (CA INDEX NAME)

ANSWER 96 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN
1981:569267 CAPLUS
95:169267
95:28301a,28304a
Studies of organosilicon compounds. XXIX. Reaction of hydroxyaldehydes and hydroxyketones with trialkylsilanes
Lapkin, I. 1.; Dvinskikh, V. V.
Perm. Gos. Univ., Perm. USSR
Zhurnal Obshchei Khimii (1981), 51(6), 1354-60
CODEN: ZOKHA4; ISSN: 0044-460X
Journal
Russian
CASREACT 95:169267
Fifteen benzyloxysilanes were prepared in 27-79% yields by the title reaction in the presence of Ni. Thus, heating p-HOC6H4CHO with Et35iH in C6H6 at 85-90° 2.5-3 h in the presence of colloidal Ni gave 59%
PHOC6H4CH2OSiEt3.
79523-76-5P
RL: SPN (Synthetic preparation): PREP (Preparation)
(preparation of)
19523-76-5 CAPLUS
Butanedioic acid, 2,3-bis(4-methylphenyl)-2,3-bis[(triethylsilyl)oxy]-, diethyl ester (9CI) (CA INDEX NAME) AU CS SO ΙT

L4 ANSWER 98 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1981:30534 CAPLUS
DN 94:30534
OREF 94:5031a,5034a

TI Electrochemical oxidation of aromatic ethers. Part 6. Oxidation of 4-(3,4-dimethoxybenzyl)-6,7-dimethoxy-2-methyl-1,2,3,4-tetrahydroisoquinoline and attempted synthesis of 4-(3,4-dimethoxybenzyl)-6,7-dimethoxy-2-methyl-1,4-dihydro-3(2H)-isoquinolone

AU Carmody, Maurice P.; Sainsbury, Halcolm: Newton, Roger F.

Sch. Chem., Univ. Bath, Bath, BAZ 7AY, UK

Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1980), (9), 2013-20

CODEN: JCPRB4; ISSN: 0300-922X

DT Journal

LA English
GI

Anodic oxidation at 1.15 and 1.9 V, resp., of the title tetrahydroisoquinoline (Bu4NBF4, CF3COZH-CH2CI2, C-felt anode, .apprx.3 h) gave the dihydroisoquinolinium derivs. I (R = H, RZ = bond, resp.), and no aryl-aryl coupled products were isolated. It is suggested that to achieve intramol. coupling of the 2 methoxylated rings their oxidation potentials should be closely similar. Cyclization of the amide II (Et polyphosphoric ester, 140°, 15 min) gave the dibenzocycloheptene III (71%), and not the expected title dihydroisoquinolone. 76056-00-3P
REL RCT (Reactant): SPN (Synthetic preparation): PREP (Preparation): RACT (Reactant or reagent)

- ANSWER 99 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1980:532199 CAPLUS 93:132199 93:21069a,21072a

- AU

- 93:132199
  93:21059a,21072a
  Thallium in organic synthesis. 57. Reaction of chalcones and chalcone ketals with thallium(III) trinitrate
  Taylor, Edward C.; Conley, Richard A.; Johnson, David K.; McKillop,
  Alexander: Ford, Michael E.
  Dep. Chem., Princeton Univ., Princeton, NJ, 08540, USA
  Journal of Organic Chemistry (1980), 45(17), 3433-6
  CODEN: JOCEAH; ISSN: 0022-3263
  Journal English
  CASREACT 93:132199
  Treatment of chalcones ArCH:CHCOAr' with Tl(NO3)3 in acidic MeOH or in
  HC(OMe)3 gave (MeO) 2CHCHArCOAr' (oxythallation-rearrangement) and/or
  MeOCHArCHAr'CO2Me (ketalization-oxythallation-rearrangement) The effect
  of substituents on Ar and Ar' on the ratio of the above rearrangement
  Troducts was examined
  74007-60-6F
  RL: SPN (Synthetic preparation); PREP (Preparation)
  (preparation of)
  74007-60-6 CAPLUS
  Benzenepropanoic acid, B-methoxy-4-methyl-α-(4-methylphenyl)-,
  methyl ester (CA INDEX NAME) IT

- ANSWER 98 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) (prepn. and cyclization of) 76056-00-3 CAPLUS
  Benzenepropanoic acid, a-[2-(bromomethyl)-4,5-dimethoxyphenyl]-3,4-dimethoxy-, ethyl ester (CA INDEX NAME) RN CN

- DN OREF TI
- ANSWER 100 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1980:516183 CAPLUS 93:116183 93:116183 93:116183 93:1612a Synthesis of trimeric lignin model compound composed of β-0-4 and β-1 structures Namba, Hiroaki; Nakatsubo, Fumiaki; Higuchi, Takayoshi Wood Res. Inst., Kyoto Inst., Uji, 611, Japan Mokuzai Gakkaishi (1980), 26(6), 426-31 CODEN: MXGAG7; ISSN: 0021-4795 Journal English

- CS SO
- English

Trilignol (I) [13459-21-7], a major structure in lignin, was synthesized in 464 overall yield via reaction of Me 4-benzyloxy-5-methoxybenzeneacetate [16209-54-4] with erythro-4-[[4-(4-benzyloxy-3-methoxybenz]-2,2-dimethy]-1,3-dioxan-5-y-jloxy]-3-methoxybenzaldehyde [74613-61-9] (5 steps), and its structure was elucidated by chemical anal. and UV. IR, NMR, and mass spectroscopy.

74613-58-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and acetylation of)
74613-58-4 CAPLUS
Benzenepropanoic acid, β-hydroxy-4-[2-hydroxy-2-(4-hydroxy-3-methoxyphenyi]-1-(hydroxymethyl) ethoxy)-α-(4-hydroxy-3-methoxyphenyi)-1-hoxy-, methyl ester (CA INDEX NAME)

ANSWER 100 OF 146 CAPLUS COPYRIGHT 2007 ACS On STN

CASREAT 93:114097

4-RCGHACHCOOZET (R = H, Me, Cl, Me2CH, Me2CHCH2) added to 22 RICH:NCGH4R2
(I; Rl = 4-Me2CHCGH4, 3,4-methylenedioxyphenyl, 2- and 4-ClCGH4, Ph,
4-FCGH4, 2-furyl; R2 = 4-Me, H, 3-Cl, 4-Cl, 3,4-methylenedioxy, 4-COZET)
in anhydrous Me2SO containing EtONa at room temperature to give 26
esponding
4-RCGH4CHCCGZET)CHRINHCGH4R2 (II) in 28-81% yield. Theor., 4-RCGH4CH2COZH
(R = H, OZN, Cl) added to 9 RICH:NR3 (Rl = Ph, 3,4-methylenedioxyphenyl,
4-Me2CHCGH4, 4-ClCGH4; R3 = Me, CGMe2, Bu) at 100° under N to give
9 corresponding 4-RCGH4CH(COZH)CHRINHR3 (III) in 11-50% yield. I (Rl =
4-ClCGH4, 4-MeZCHCGH4, RZ = 3,4-methylenedioxy; Rl = 4-MeZCHCGH4, RZ = 3, body weight II (R = H, Cl, Rl = 3,4-methylenedioxyphenyl, R2 = H, 4-Me, 4-Cl; R = R2 = H, Rl = 4-Me2CHCGH4) and III (R = H, Rl = 3,4-methylenedioxyphenyl, R3 = CHMe2, Bu; R = Cl, Rl = 4-Me2CHCGH4, R3 = Me) had weak antiinflammatory activity.

74760-33-1P

(preparation, toxicity and antiinflammatory activity of)

74760-33-1 CAPLUS

Benzenepropanoic acid, 4-(1-methylethyl)-α-(4-methylphenyl)-β-(phenylamino)-, ethyl ester (CA INDEX NAME)

ANSWER 101 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1980:516113 CAPLUS 93:116113 93:18601a,18604a Poly(vinyl chloride) plastisol compositions Dainippon Ink and Chemicals, Inc., Japan Jpn. Rokai Tokkyo Koho, 5 pp. CODEN: L4 AN DN OREF TI PA SO DT Patent LA Japanese FAN.CNT 1 ONT 1 PATENT NO. KIND DATE APPLICATION NO. DATE JP 55052335 19800416 JP 1978-125721 19781014 PΙ JP 61047868 PRAI JP 1978-125721 GI 19861021 19781014

PVC [9002-86-2] plastisols containing I (R = CN, COZR1; R1 = C1-3 alky1) as radical initiators gave baked coatings free from bubbles. For example, a PVC plastisol containing trimethylolpropane trimethacrylate [3290-92-6] (reactive plasticizer) 60, DOP 100, epoxidized soybean oil 3, CaCO3 200, a Sn stabilizer 2, and I (R = CN, R1 = Me) (II) [31249-03-3] 12 phr was baked on tinplate at 120\* to give a coating with better adhesion and lower bubble content than that using 1,1-bis(tert-butylperoxy)-3,3,5-trimethylcyclohexane in place of II. 31249-03-3

31249-03-3
(catalyst use): USES (Uses)
(catalysts, for crosslinking of PVC plastisol coatings)
31249-03-3 CAPLUS
Butanedioic acid, 2,3-dicyano-2,3-bis(4-methylphenyl)-, dimethyl ester
(9CI) (CA INDEX NAME)

L4 ANSWER 103 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN AN 1980:128633 CAPLUS ON 92:128633 CAPLUS ON 15 ON DT LA GI

Phenylcoumarans I (R, R1 = H, MeO) were prepared by introducing a 2C side chain to a vanillin derivative, cyclization of the substituted vanillin to form a phenylcoumaran, and extension of the aldehyde side chain. Thus, II [R2 = idod, R3 = CH(Me)2], was treated with BULi and DMF followed by reaction with MeSCH2SOMe and methanolysis to give II (R2 = CH2COZMe, R3 = CH(CMe)2, III). III was condensed with II (R2 = H, R3 = CHO) in the presence of LiN(CHMe2) to give 80% threo-IV (R4 = COZMe). Subsequent silylation and reduction gave field IV (R4 = CHZOH). The diol was then hydrogenated and cyclized by treating with Et2O.BF3 in CHCI2. A Wittig reaction of the resulting phenylcoumaran V with 1,3-dioxan-2-ylmethyltriphenylphosphonium bromide followed by NaBH4 reduction gave I (R = H, R1 = CMe) in 90% overall yield.
73022-32-99
RL: RCT (Reactant): SPN (Synthetic preparation): PREP (Preparation): RACT (Reactant or reagent) (preparation and reduction of)
73022-32-9 CAPUS
Benzenepropanoic acid, o-(5-(dimethoxymethyl)-3-methoxy-2-(phenylmethoxyl)phenyl]-3-methony-4-(phenylmethoxyl)-B-(trimethylsilyl)oxy)-, methyl ester, (R\*,S\*)- (9CI) (CA INDEX NAME)

ANSWER 103 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN Relative stereochemistry.

73022-30-7P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and silylation of)
73022-30-7 CAPLUS

73022-30-7 CAPLUS
Benzenepropanoic acid, a-[5-(dimethoxymethyl)-3-methoxy-2(phenylmethoxy)phenyl]-β-hydroxy-3-methoxy-4-(phenylmethoxy)-, methyl
ester, (R\*,S\*)- (9Cl) (CA INDEX NAME)

Relative stereochemistry.

ANSWER 104 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN ester (9CI) (CA INDEX NAME)

ANSWER 104 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1979:473877 CAPLUS 91:73877 91:11933a,11936a Bimolecular self-reactions of 2-arylindandion-1,3-yl radicals studied by flash photolysis Khudyakov, I. V.; Yasmenko, A. I.; Kuz'min, V. A. Inst. Chem. Phys., Moscow, 117334, USSR International Journal of Chemical Kinetics (1979), 11(6), 621-33 CODEN: IJCKBO; ISSN: 0538-8066 Journal English CS SO

Kinetic and thermodn, data for the title reaction of aromatic radicals I [R Kinetic and thermodn. data for the title reaction of aromatic radicals I [R H. Rl = NMe2 (II); R = H.Rl = NEt2 (III); R = H.Rl = NPr2 (IV); R = H. Rl = NBu2 (V); R = H. Rl = NPr2 (VI); R = Rl = OMe (VII); R = Br, Rl = NMe2 (VIII)], IX, X, and XI were obtained. The recombination reactions in volving radicals II-V are limited by diffusion in solvents having a viscosity n < 10cP and are activation reactions in solvents having a viscosity n < 10cP. The recombination of radicals IX and X is an activation reaction, while that of radicals VI-VIII is diffusion-controlled in the entire viscosity range. The recombination of radicals XI is limited, in the viscosity range of 18.4 to 2 cP, by intrusion into the first coordination sphere of the partner, the effect of viscosity on the radical XI recombination rate in the specified range being the same as its effect on diffusion-controlled reactions. The possible reasons of the discrepancies between the exptl. fast recombination rate consts. and the theor. values calculated by the Debye-Smoluchowski theory are discussed. The equilibrium constant depends strongly on the nature of the substituent in the Ph fragment: the substituents which increase unpaired electron delocalization in the radical intensify the dissociation of the resp. dimer.

71023-19-3

/10/2-19-3 (dissociation of) 1702-19-3 CAPLUS Butanedioic acid, 2,3-dicyano-2,3-bis(2,4,6-trimethylphenyl)-, diethyl

ANSWER 105 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1979:419465 CAPLUS
DN 91:19465 CAPLUS
DN 91:19465 CAPLUS
DN 91:19465 CAPLUS
TI Voltammetric study of the anodic oxidation of enclate carbanions
AU Kern, Jean Marc: Federlin, Paul
CS Inst. Chim., Univ. Louis Pasteur, Strasbourg, 67000, Fr.
SO Journal of Electrocanalytical Chemistry and Interfacial Electrochemistry (1978), 96(2), 209-28
CODEN: JEIEBC; ISSN: 0022-0728
DT Journal
LA English
AB A voltammetric study of the anodic oxidation of the enclate carbanions of B-ketonitriles RCH(CN)COR1 has been carried out in Me2SO. The variation of Eos of these species as a function of the nature of R and R1 vas examined Their anodic oxidation process could be identified by analthe voltampercentric curves obtained both at the rotated Pt electrode and at the stationary electrode. Cyclic voltammetry has confirmed that this is an ec overall irreversible process. The electrochem: reaction e yielding a neutral radical is followed by the very fast dimerization (2nd-order chemical reaction c). The formation of different kinds of dimers, depending on the nature of the oxidized enolates, has been observed during depending on the nature of the oxidized enolates, has been observed during

(2nd-order chemical reaction u). The constant of the control of the property of the control of t

L4	ANSWER 106 OF 146	CAPLUS	COPYRIGHT	2007 ACS on STN	
AN	1979:203702 CAPLUS	5			
DN	90:203702				
OREF	90:32393a,32396a				
TI	5-Oxopentanoic acid	deriv	atives		
IN				Grimova, Jaroslava	
PA	Czech.		•		
so	Czech., 6 pp.				
	CODEN: CZXXA9				
DT	Patent				
LA	Czech				
FAN.	CNT 1				
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	CS 176744	B1	19770630	CS 1975-2824	19750423
PRAI	CS 1975-2824	Α	19750423		
GI					

The title compds. I (R1 = H, C3-4 alkyl, Cl, NO2, OMe: R2 = H, CHMe2, NMe2, Cl, NO2: R3 = Ph, 2-furyl, OMe3, 3-indanyl, C6H3C12-2,4) were prepared by addition of 4-RIC6H4CH2CO2Et to 4-R2C6H4CH:CHCOR3 and saponification of

product. Thus, a solution of 2.46 g PhCH2CO2Et and 3.7 g
4-Me2CHC6H4CH:CHCOPh in Et20 containing EtONa was kept 5 days to give 4.4 g
PhCOCH2CH(CGH4CHW62-4)CHPhCO2Et which was refluxed with AcOH-HBr to yield
3.5 g I (R1 = H, R2 = CHMe2, R3 = Ph). Similarly prepared were
PhCOCH2CH4CH8CO2H (R4 = 2-pyrrolyl, 3-pyridyl; R5 = Ph, CGH4NO2-4,
CGH4CH2CHW62-4).

59771-47-0P 70334-43-9P 70334-45-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
59771-47-0 CAPLUS
Benzenepentanoic acid, B-[4-(1-methylethyl)phenyl]-α-[4-(1-methylpropyl)phenyl]-6-oxo-, ethyl ester (9CI) (CA INDEX NAME)

70230-43-2 CAPLUS Butanedioic acid, 2,3-dicyano-2,3-bis(4-methylphenyl)-, 1,4-diethyl ester (CA INDEX NAME)

70245-03-3 CAPLUS Butanedioic acid, 2,3-dicyano-2,3-bis(4-methylphenyl)-, ethyl methyl ester (9C1) (CA INDEX NAME)

ANSWER 106 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN

(Continued)

70334-43-9 CAPLUS

Benzenepropanoic acid, B-(3,3-dimethyl-2-oxobutyl)-4-(1-methylethyl)-a-[4-(2-methylpropyl)phenyl]-, ethyl ester (CA INDEX NAME)

70334-45-1 CAPLUS Benzenepropanoic acid,  $\beta$ -{3,3-dimethyl-2-oxobutyl}-4-(1-methylethyl)- $\alpha$ -{4-(1-methylethyl)phenyl}-, ethyl ester (CA INDEX NAME)

ANSWER 107 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

70245-07-7 CAPLUS
Butanedioic acid, 2,3-dicyano-2-[4-methyl-2-[(methylthio)methyl]phenyl]-3-(4-methylphenyl)-, dimethyl ester (9CI) (CA INDEX NAME)

70245-08-8 CAPLUS

Butanedioic acid, 2.3-dicyano-2-[4-methyl-2-[(methylthio)methyl]phenyl]-3-[4-methyl-3-[(methylthio)methyl]phenyl]-, dimethyl ester (9CI) (CA INDEX NAME)

The structure of the spermine alkaloid aphelandrine from Aphelandra The structure of the spermine alkalold appelanding from appelanding aquarrons Nees
Daetwyler, Peter: Bosshardt, Herbert; Bernhard, Heinz O.; Hesse, Manfred;
Johne, Siegfried
Org.-Chem. Inst., Univ. Zurich, Zurich, Switz.
Helvetica Chimica Acta (1978), 61(7), 2646-71
CODEN: HCACAV: ISSN: 0018-019X ΑU DT LA GI Journal German

í.

The structure of aphelandrine from A. squarrosa was determined to be I from chemical and spectral data.
69721-65-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
69721-65-9 CAPLUS
Benzenepropanoic acid, α-[2-hydroxy-5-(3-methoxy-3-oxopropyl)phenyl]-4-methoxy-, methyl ester (CA INDEX NAME)

ANSWER 109 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

ANSWER 109 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1979:103658 CAPLUS 90:103658 90:103658 90:16366a 90:16363a,16366a Substituted phenylacetonitrile Maurer, Manfred; Lange, Fritz Walter: Orth, Winfried; Miele, Heinrich: Fickert, Werner Ruetgerswerke A.-G., Fed. Rep. Ger. Ger. Offen., 26 pp. CODEN: GWXXEX Patent DT Pate. LA German FAN.CNT 1 PATENT NO. APPLICATION NO. DATE KIND DATE 19780831 19770225 A1 B2 C3 DE 1977-2708142 DE 2708142
DE 2708142
DE 2708142
ES 462366
CH 632236
FR 2381750
PRAI DE 1977-2708142 19800918 19811029 19780601 ES 1977-462366 19770914 19820930 CH 1977-15344 FR 1978-4716 19771213 19780220 19780922 19770225 MARPAT 90:103658

Substituted phenylacetonitriles I (R.= Cl-4 alkyl, C5-7 cycloalkyl or benzyl, optionally substituted by Br, Cl or carbalkoxy: Rl and R2 = Cl-4 alkyl) and 3-H02CCGH4CHRCN (II, R = same as in I) were prepared Thus, 3-Me02CCGH4CH2CH created successively with NaCN, Na and Me0COZMe gave 3-Me02CCGH4CNa(CN)COZMe which, treated with Me2S04 gave I (R = R1 = R2 = Me), which was saponified and partially decarboxylated to give II (R = Me). 68433-08-9P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation, saponification and partial decarboxylation of) 68433-08-9 CAPLUS Benzenepropanoic acid, 4-chloro-α-cyano-α-[3-(ethoxycarbonyl)phenyl]-, ethyl ester (CA INDEX NAME) IT

ANSWER 110 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1979:38643 CAPLUS 90:38643 (APLUS 90:38643 SP. 90:58613 (APLUS 90:38643 SP. 90:6219a Reaction of carbanion of pentafluorophenylcyanoacetic ester with electrophilic reagents Zakharova, O. V.; Vlasov, V. M.; Yakobson, G. G. Novosib. Inst. Org. Khim., Novosibirsk, USSR Zhurnal Organicheskoi Khimii (1978), 14(9), 1895-904 (CODEN: ZORKAE; ISSN: 0514-7492 Journal Russian (GFSC-(CN)COZEt ISSN: 0514-7492 Journal Russian (GFSC-(CN)COZEt I), and at 95-150° to 5644 (GFSCHICR) via (GFSC-HCN) And HOLD (GFSC-HCN) And HOLD (GFSC-HCN) (OZET (1), and at 95-150° to 5644 (GFSCHICR) via (GFSC-HCN) Na+ and/or (GFSC-HCN) Na+ 1010 (FSC-HCN) Na+ and/or (GFSC-HCN) Na+ 1010 (FSC-HCN) Na+ (HZ)CHCN (in Et3N at 70 and 130° gave (GFSCH(CN)CHZCHZC) (R1 - COZEt, H, resp.). Treating II with CF2:CFCF3 gave (GFSCH(CN)CHZCHZCN) (R1) (HZCHZCN, CL) gave 40-731 (GFSCHRCOZH. GFSSB-75-4P RL): SNN (Synthetic preparation); PREP (Preparation) (preparation of (6598-75-4 CAPLUS) Benzenepropanoic acid, a-cyano-2,3,4,5,6-pentafluoro-α-(pentafluorophenyl)-, ethyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 111 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1979:6107 CAPLUS
DD 90:6107
OREF 90:1109a,1112a
T1 3-Carboxyphenylacetic acid derivatives
IN Haurer, Manfred; Lange, Fritz Walter; Orth, Winfried; Miele, Heinrich; Fickert, Werner
FA Ruetgezwerke A.-G., Fed. Rep. Ger.
SO Ger. Offen. 25 pp.
CODEN: GWXXBX
DT Patent
L4 German

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2708143	A1	19780831	DE 1977-2708143	19770225
DE 2708143	B2	19800626		
DE 2708143	C3	19811119		
NL 7713112	Α	19780829	NL 1977-13112	19771129
ES 464851	A1	19780801	ES 1977-464851	19771207
AT 7801340	A	19790515	AT 1978-1340	19780224
AT 353777	В	19791210		
GB 1555849	Ā	19791114	GB 1978-7732	19780227
	Ä	19770225		
	UN.CNT 1 PATENT NO. DE 2708143 DE 2708143 DE 2708143 NL 7713112 ES 464851 AT 7801340 AT 353777 GB 1555849	N.CNT 1 PATENT NO. KIND DE 2708143 A1 DE 2708143 B2 DE 2708143 C3 NL 7713112 A E5 464851 A1 AT 7801340 A AT 353777 B GB 1555849 A	N.CHT 1 PATENT NO. KIND DATE  DE 2708143 A1 19780831 DE 2708143 B2 19800626 DE 2708143 C3 1981119 ML 7713112 A 19780829 ES 464851 A1 19780829 ES 464851 A1 19790515 AT 3833777 B 19791210 GB 1555849 A 19791114	N.CHT 1 PATENT NO. KIND DATE APPLICATION NO.  DE 2708143 A1 19780831 DE 1977-2708143  DE 2708143 B2 19800626  DE 2708143 C3 1981119  NL 7713112 A 19780829 NL 1977-13112  ES 464851 A1 19780801 ES 1977-464851  AT 7801340 A 19790515 AT 1978-1340  AT 353777 B 19791210  GB 1555849 A 19791114 GB 1978-7732

68433-08-99 CAPLUS

68433-08-9 CAPLUS

b8433-U8-9 CAPLUS Benzenepropanoic acid, 4-chloro-α-cyano-α-[3-(ethoxycarbonyl)phenyl]-, ethyl ester (CA INDEX NAME)

(Continued) ANSWER 112 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN

59667-04-8 CAPLUS Benzenepropanoic acid, 2,6-dichloro- $\alpha$ -(4-chlorophenyl)-, ethyl ester (CA INDEX NAME)

59667-13-9 CAPLUS Benzenepropanoic acid, 2,4-dichloro- $\alpha$ -(2,6-dichlorophenyl)-, methyl ester (CA NNDEX NAME)

59667-14-0 CAPLUS Benzenepropanoic acid, 4-chloro-q-(2,6-dichlorophenyl)-, methyl ester (CA INDEX NAME)

59667-36-6 CAPLUS Benzenepropanoic acid, 4-chloro- $\alpha$ -(2-chlorophenyl)-, methyl ester (CA INDEX NAME)

ANSWER 112 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN

1977:601405 CAPLUS

L4 ANSWER 112 OF 144 AN 1977:601405 CAP DN 87:201405 OREF 87:31887a,31890a TI Antimycotic imid: 87:31887a,31890a
Antimycotic imidazoles. 2. Synthesis and antimycotic properties of l-[2-(arylalkyl)-2-phenylethyl]-1H-imidazoles
Heeres, Jan; Hostmans, Jozef H.: Van Cutsen, Jan
Res. Lab., Janssen Pharm., Beecne. Belg.
Journal of Medicinal Chemistry (1977), 20(11), 1511-16
CODEN: JMCMAR; ISSN: 0022-2623
Journal
English
CASREACT 87:201405

1-[2-(Arylalky1)-2-phenylethy1]-1H-imidazoles I (Rn = 2-C1, -Br, -Me, 4-C1, 2,4-, 2,6-C12; Rln = H, 2-, 4-C1, 4-Br, -OWe, 2,4-, 2,6-C12; m = 1, 2) were prepared from the corresponding RnC6H5-nCH2CN via successive alkylation with X(CH2)mC6H5-nRin (X = halo), conversion to the corresponding ester RnC6H5-nRin (X = halo), conversion to the corresponding ester RnC6H5-nRi(CO2R) (CH2)mC6H5-nRin. These alcs. were meylated and the products refluxed with imidazole in DMF to yield I which were active in vitro against dermatophytes, yeasts, other fungi, and gram-positive bacteria. Some were also active in vivo against Candida albicans.

ΙT

gram-positive bacteria. Some were also active in vivo against Candida albicans.

59667-03-7P 59667-04-8P 59667-13-9P
59667-14-0P 55667-36-6P 59667-38-8P
64008-30-6P 64008-31-7P 64008-32-8P
64008-39-5P 64008-31-7P 64008-35-1P
64008-39-5P 64008-7-37-9 64008-38-4P
64008-39-5P 64008-40-8P 64008-41-9P
64008-40-0P 64008-44-2P'
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)
59667-03-7 CAPLUS
Benzenepropanoic acid, 2,4-dichloro-q-(2-chlorophenyl)-, methyl

Benzenepropanoic acid, 2,4-dichloro-q-(2-chlorophenyl)-, methyl ester (CA INDEX NAME)

ANSWER 112 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

59667-38-8 CAPLUS Benzenepropanoic acid, 2,6-dichloro- $\alpha$ -(2-chlorophenyl)-, methyl ester (CA INDEX NAME)

64008-30-6 CAPLUS Benzenepropanoic acid, 2,4-dichloro-α-(2-methylphenyl)-, methyl ester (CA INDEX NAME)

64008-31-7 CAPLUS Benzenepropanoic acid, 2,6-dichloro- $\alpha$ -(2-methylphenyl)-, methyl ester (CA INDEX NAME)

64008-32-8 CAPLUS Benzenepropanoic acid, 4-chloro-a-(2-methylphenyl)-, methyl ester (CA INDEX NAME)

ANSWER 112 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN

64008-33-9 CAPLUS Benzenepropanoic acid, 2-chloro-a-(2-chlorophenyl)-, methyl ester (CA INDEX NAME)

64008-34-0 CAPLUS Benzenepropanoic acid, α-(2-bromophenyl)-2,4-dichloro-, methyl ester (CA INDEX NAME)

64008-35-1 CAPLUS Benzenepropanoic acid,  $\alpha$ -(2-bromophenyl)-4-chloro-, methyl ester (CA INDEX NAME)

64008-36-2 CAPLUS Benzenepropanoic acid, 2-chloro- $\alpha$ -(4-chlorophenyl)-, ethyl ester (CA INDEX NAME)

ANSWER 112 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

64008-41-9 CAPLUS Benzenepropanoic acid, 2,6-dichloro-α-(2,4-dichlorophenyl)-, ethylester (CA INDEX NAME)

64008-42-0 CAPLUS Benzenepropanoic acid, 4-bromo-α-(2,4-dichlorophenyl)-, methyl ester (CA INDEX NAME)

64008-44-2 CAPLUS Benzenepropanoic acid, q-(2,4-dichlorophenyl)-4-methoxy-, methyl ester (CA INDEX NAME)

ANSWER 112 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN

64008-37-3 CAPLUS Benzenepropanoic acid, 2,4-dichloro- $\alpha$ -(4-chlorophenyl)-, ethyl ester (CA INDEX NAME)

64008-38-4 CAPLUS Benzenepropanoic acid, 2-chloro-a-(2,4-dichlorophenyl)-, methyl ester (CA INDEX NAME)

64008-39-5 CAPLUS Benzenepropanoic acid, 4-chloro- $\alpha$ -(2,4-dichlorophenyl)-, ethyl ester (CA INDEX NAME)

64008-40-8 CAPLUS Benzenepropanoic acid, 2,4-dichloro- $\alpha$ -(2,4-dichlorophenyl)-, ethyl ester (CA INDEX NAME)

L4 ANSWER 113 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1977:72650 CAPLUS DN 86:72650 CAPLUS DN 86:72650 The first of the fi

LA FAN	LA English FAN.CNT 2								
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE.				
PI	US 3991201	Α	19761109	US 1975-578777	19750519				
	US 3927017	Α	19751216	US 1974-483587	19740627				
PRA	I US 1974-483587	A3	19740627						

Arylethylimidazoles I (R = 4-FC6H4, 4-C1C6H4, 2-C1C6H4, 2,4-C12C6H3, 2,6-C12C6H3, Ph; R1 = C1-8 alkyl, allyl, 2-C1C6H4CH:CHCH2, chlorobenzyl, bromobenzyl, cyclohexyl, cyclopentyl, 4-MeOC6H4CH2, 4-MeC6H4CH2) (55 compds.) were prepared by treating RCH2CN with R1Br, hydrolyzing RRICHCN, esterifying RRICHCO2H, LiRH4 reduction of RRICHCO2Me, treatment of MCH2CH4 RR1CHCH2OH

HCH2OH
with MeSO3H, and treatment of RRICHCH2O3SMe with imidazole.
59667-13-9P
RL: RCT (Reactant): SPN (Synthetic preparation); PREP (Preparation): RACT
(Reactant or reagent)
(preparation and reduction of)
59667-13-9 CAPLUS

Benzenepropanoic acid, 2,4-dichloro-a-(2,6-dichlorophenyl)-, methyl ester (CA INDEX NAME)

IT

59667-03-7P 59667-04-8P 59667-14-0P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of) 59667-03-7 CAPUS Benzenepropanoic acid, 2,4-dichloro-a-(2-chlorophenyl)-, methyl ester (CA INDEX NAME)

ANSWER 113 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

59667-04-8 CAPLUS

Benzenepropanoic acid, 2,6-dichloro-e-(4-chlorophenyl)-, ethyl ester (CA INDEX NAME)

59667-14-0 CAPLUS

Benzenepropanoic acid, 4-chloro- $\alpha$ -(2,6-dichlorophenyl)-, methyl ester (CA INDEX NAME)

L4 ANSWER 115 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1976:446150 CAPLUS
DN 85:46150
RF 85:7487a, 7490a
T1 The erythro and threo isomers of 2,3,4-substituted butanoic acids
AV Fisnerova, L.; Kakac, B.; Kraus, E.; Nemecek, O.
Res. Inst. Pharm. Biochem., Prague, Czech.
COLECTION CZECACK; ISSN: 0010-0765

Journal English CASREACT 85:46150

DT LA OS GI

# - CH (CO2R3) CHR1CH2COR

Title compds. I (R = Ph, Me3C; R1 = Ph, 4-Me2NC6H4, 4-Me2CHC6H4, 4-ClC6H4, 4-OiNC6H4, 3-pyridyl, 4-Me0CGH4, 2-pyrrolyl; R2 = H, NO2, Me2CHCH2, EtCHMe, Me2CH, Cl, Me0; R3 = H, Et) were prepared and tested for antiinflammatory activity. I were prepared by reaction of RCOCH:CHR1 and p-R2CGHCH2CO2R3 catalyzed by NaNH2 in NH3 (I) for R3 = H and by EtCNa in Et2O for R3 = Et. Some I (R3 = H) were prepared by hydrolysis of the corresponding I (R3 = Et) in boiling AcOH-HBr. The threo isomers were obtained by the NaNH2-NH3(I) method or by epimerization of the erythro isomers via enol lactones. The highest antiinflammatory activity was found in I (R = Ph, R1 = 3-pyridyl, R2 = Me2CHCH2, R3 = H) and I (R = Ph, R1 = 4-Me2CHGH4, R2 = R3 = H) (II). The effect of configuration on the antiinflammatory activity was also studied: threo-II was .apprx.15% more active than erythro-II.

59771-47-UP 59771-65-IP 59771-65-P
59771-10-DF

59771-71-0P
RE: RCT (Reactant): SPN (Synthetic preparation): PREP (Preparation): RACT (Reactant or reagent)
(preparation and hydrolysis of)
59771-47-0 CAPLUS
Benzenepentanoic acid, %-[4-{]-methylethyl]phenyl]-a-[4-{]-methylpropyl)phenyl]-8-0xo-, ethyl ester (9CI) (CA INDEX NAME)

59771-64-1 CAPLUS
Benzenepentanoic acid, α,β-bis[4-(1-methylethyl)phenyl]-δ-oxo-, ethyl ester, {R\*,R\*}- (9CI) (CA INDEX NAME)

L4 ANSWER 114 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1976:477455 CAPLUS
DN 85:77455
CREF 85:12445a,12448a
TI Effect of substituents on the stereochemistry of the Reformatskii reaction
AU Hladenova, M.: Blagoev, B.: Kurtev, B.
CS Inst. Org. Chem., Sofia, Bulg.
CD Doklady Bolgarskoi Akademii Nauk (1975), 28(12), 1633-6
CODEN: DBANAD: ISSN: 0366-8681
DT Journal
LA French

Journal
French
The Reformatskii reaction of RC6H4CH0 (R = H, p-Me, o-Me, p-Cl, o-Cl, p-MeO) and 1-naphthaldehyde with p-RIC6H4CHDrOZMe (R1 = Br, H) gave an apprx.80:50 mixture of erythro- and three-RC6H4CH(M) CH(GCHRAI-p)COZMe or the 1-naphthyl analog in Et2O. In (MeO)ZCHZ, the erythro-isomer was slightly favored (.apprx.60:40); in MeZSO, the three isomer was favored (.apprx.70:30). In MeZSO, p-RIC6H4CH(COZMe)CH(COZMe)CHHR-p was also formed. The lack of substituent effects in the Reformatskii reaction was explained by a transition state resembling the starting materials. 60079-94-9P
RL: SPN (Synthetic preparation): PREP (Preparation) (preparation of) 60079-94-9 CAPLUS
Butanedioic acid, 2,3-bis(4-bromophenyl)-, dimethyl ester (9CI) (CA INDEX NAME) ΙT

L4 ANSWER 115 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

Relative stereochemistry.

59771-65-2 CAPLUS

Benzenepentanoic acid, α,β-bis[4-(1-methylethyl)phenyl]-5-oxo-, ethyl ester, (R\*,S\*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

59771-68-5 CAPLUS
Benzenepropanoic acid, β-(3,3-dimethyl-2-oxobutyl)-4-(1-methylethyl)α-[4-(2-methylpropyl)phenyl}-, ethyl ester, (R\*,R\*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

59771-69-6 CAPLUS
Benzenepropanoic acid, β-(3,3-dimethyl-2-oxobutyl)-4-(1-methylethyl)-α-(4-(2-methylpropyl)phenyl)-, ethyl ester, (R\*,5\*\Lambda-(9CI) (CA

Relative stereochemistry.

ANSWER 115 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN

59771-70-9 CAPLUS Benzenepropanoic acid, β-{3,3-dimethyl-2-oxobutyl}-4-(1-methylethyl)-a-[4-(1-methylethyl)phenyl]-, ethyl ester, (R\*,R\*)- (9CI) (CA INDEX

Relative stereochemistry.

$$i-Pr$$

$$0$$

$$0$$

$$Et$$

$$1-Bu$$

$$0$$

$$Pr-i$$

59771-71-0 CAPLUS Benzenepropanoic acid,  $\beta$ -(3,3-dimethyl-2-oxobutyl)-4-(1-methylethyl)- $\alpha$ -[4-(1-methylethyl)phenyl]-, ethyl ester,  $(R^*,S^*)$ -(9CI) (CA INDEX

Relative stereochemistry.

ANSWER 116 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Conti 59667-03-7 CAPLUS Benzenepropanoic acid, 2,4-dichloro-a-(2-chlorophenyl)-, methyl ester (CA INDEX NAME)

59667-04-8 CAPLUS Benzenepropanoia caid, 2,6-dichloro- $\alpha$ -(4-chlorophenyl)-, ethyl ester (CA INDEX NAME)

59667-14-0 CAPLUS
Benzenepropanoic acid, 4-chloro-q-(2,6-dichlorophenyl)-, methyl
ester (CA INDEX NAME)

59667-36-6 59667-37-7 59667-38-8
RL: RCT (Reactant): RACT (Reactant or reagent)
(reduction of)
59667-36-6 CAPUS
Benzenepropanoic acid, 4-chloro-a-(2-chlorophenyl)-, methyl ester
(CA INDEX NAME)

59667-37-7 CAPLUS

L4 ANSWER 116 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN N 1976:433007 CAPLUS N 8:33007 CAPLUS N 8:33007 CAPLUS N 8:33007 CAPLUS N 19:3000 DT Patent LA English FAN.CNT 2 PATENT NO. KIND DATE APPLICATION NO. DATE PI US 3927017 US 3991201 PRAI US 1974-483587 GI 19751216 19761109 19740627 US 1974-483587 US 1975-578777

Imidazoles I [Rn = Cl, F, H, 2,4-, 2,6-Cl2: Rl = alkyl, allyl, cycloalkyl, CH2CGH5R2,CH2CGH4Cl2-2,4, CH2CGH4Cl2-2,6: R2 = Cl, Br, 4-Me, 4-MeO, CH2CH2Ph] (53 compds.), fungicides, bacteriostats, and bactericides at 0.1-100 y/ml, were prepared by treating benzeneacetonitriles II (R3 = H) with halides RIX, hydrolyzing-esterifying II (R3 = R1) with HCl in MeOH or EtOH, reducing the ester RnCGH5-nCHR1CQ2A4 (R4 = Me, Et) with NaBH4 over LiX in MeCN, mesylating the alc. RnCGH5-nCHR1CH2OH, and treating the methanesulfonate with imidazole.

59667-13-99

59667-13-9P
RL: RCT (Reactant): SPN (Synthetic preparation): PREP (Preparation): RACT (Reactant or reagent) (preparation and reduction of) 59667-13-9 CAPLUS Benzenepropanoic acid, 2,4-dichloro-a-(2,6-dichlorophenyl)-, methyl ester (CA INDEX NAME)

59667-03-7P 59667-04-8P 59667-14-0P RL: SPN (Synthetic preparation): PREP (Preparation) (preparation of) ΙT

ANSWER 116 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) Benzenepropanoic acid, 2-bromo-a-(2,4-dichlorophenyl)-, methyl ester (CA INDEX NAME)

59667-38-8 CAPLUS Benzenepropanoic acid, 2,6-dichloro- $\alpha$ -(2-chlorophenyl)-, methyl ester (CA INDEX NAME)

L4 ANSWER 117 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1974:426419 CAPLUS
DN 81:26419
OREF 81:42653,4269a
TI Testing procedure for catalysts in polyester moldings
Al Simmonds, John; Roskott, L.
CS Novadel Ltd., Gillingham/Kent, UK
Proceedings of the Annual Conference - Reinforced Plastics/Composites
Institute, Society of the Plastics Industry (1973), 28, 1C, 12 pp.
CODEN: PCRPBG: ISSN: 0160-9750
DT Journal
LA English
AB The most useful tests were determination of the time to peak exotherm of pure

pure polyester and of molding compound and determination of shrinkage as measured by a displacement meter, which indicated min. molding time, and the kick-off time (where the kick-off temperature showed a marked diversion from the warming-up curve, which was a measure of gel time. Also valuable were residual styrene [100-42-5] determination, indicating degree of curing, and

Warming-up curve, which can be residual styrene [100-42-5] determination, indicating degree of curing, and gloss determination by a gloss meter (DIM 67530), the main parameter by which the appearance of the product was judged. Four different peroxide types, i.e., benzoyl peroxide [9-4-36-0], tert-butyl peroxide [9-2-ethyl hexanoate [3006-82-4], 1,1-bis(tert-butyl peroxy)-3,3,5-trimethylcyclohexane [6731-36-8], and (m-phenylene disopropylidene) bis[tert-butyl peroxide] [2212-81-9] were used as initiators, and the test methods also predicted the performance of a bibenzyl or G-C initiator, 1,2-bis[p-methylphenyl)-1,2-dimethoxycarbonyl-1,2-dicyanoethane [31249-03-3].

II 31249-03-3
RL: CAT (Catalyst use): USES (Uses)
(catalyst, for crosslinking of unsatd. polyester molding compound, evaluation of)
RN 31249-03-3 CAPLUS
CN Butanedioic acid, 2,3-dicyano-2,3-bis(4-methylphenyl)-, dimethyl ester (9CI) (CA INDEX NAME)

ANSWER 119 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1974:84002 CAPLUS DN 80:84002
OREF 80:13533a,13536a
TI Evaluating cataly
AU Simmonds, J.; Ros
CS Novadel Ltd., Akz
SO Modern Plastics 80:84002 SV:13333,133138
Svaluating catalysts for polyester molding compounds
Simmonds, J. Roskott, L.
Novadel Ltd., Akzo Chem. Div., Gillingham/Kent, UK
Modern Floatics (1973), SO(10), 168-9, 172, 174, 178
CODEN: MODIARY ISSN: 0026-8278 English English
Improved gloss and stability were imparted to polyester molding compds. by replacement of diacyl, perketal, peroxy ester, or dialkyl peroxide catalysts with 1,2-bis(p-methylphenyl)-1,2-dicarbomethoxy-1,2-dicyanoethane [31249-03-3].
31249-03-3 ΙT RL: USES (Uses) (catalysts for crosslinking of unsatd. polyesters)
31249-03-3 CAPLUS
Butanedioic acid, 2,3-dicyano-2,3-bis(4-methylphenyl)-, dimethyl ester
(9CI) (CA INDEX NAME)

ANSWER 118 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1974:133668 CAPLUS 80:133668 OREF 80:21561a,21564a TI Photosensitized 80:21561a,21564a
Photosensitized oxidation of an enaminoketone. Total synthesis of a rhoeadine alkaloid
Orito, K.; Manske, R. H.; Rodrigo, R.
Dep. Chem., Univ. Waterloo, Waterloo, ON, Can.
Journal of the American Chemical Society (1974), 96(6), 1944-5
CODEN: JACSAT; ISSN: 0002-7863
Journal
English
For diagram(s), see printed CA Issue.
(t) cis-Alpinine I was synthesized. Indenone intermediate II, prepared by standard methods was oxidatively rearranged in a dye-sensitized photo-oxidation process to ketolactone III which was transformed into I.
52658-50-IP
RL: SPN (Synthetic preparation): PREP (Preparation)
(preparation of) (preparation of)
52658-50-1 CAPLUS
Benzenepropanoic acid, α-[2-[2-(acetylmethylamino)ethyl]-4,5-dimethoxyphenyl]-2,3-dimethoxy-, ethyl ester (CA INDEX NAME)

L4 ANSWER 120 OF AN 1974:59616 CAI DN 80:59616 OREF 80:9665a,9668a TI Chemical struct ANSWER 120 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1974:59616 CAPLUS 80:59616

Chemical structure and sweet taste of isocoumarins and their derivatives.

IV Yamato, Masatoshi; Sato, Koichi; Hashigaki, Kuniko; Ishikawa, Tadataka; Koyama, Takaji Med. Sch., Univ. Okayama, Okayama, Japan Yakugaku Zashi (1973), 93(12), 1639-42 CODEN: YKKZAJ; ISSN: 0031-6903 ΑU

CS SO

CODEN: YKKZAJ, ISSN: 0031-6903
Journal
Japanese
For diagram(s), see printed CA Issue.
Further investigation was made on the derivs. of β-[3-hydroxy-4methoxyphenyl]ethylbenzene which is regarded as the essential structure
for the sweet taste of phyllodulcin, and compds. (I-XII) were synthesized.
Both VIII and XI were sweet, whereas II, III, and IV were tasteless, and
V, VI, VII, IX, X, and XII revealed a bitter taste. On the basis of these
data, a delicate relation between the mol. structure and sweet taste
receptor site was presumed.
51458-16-3P
RLI SPN (Synthetic preparation): PREP (Preparation)

51458-16-37
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
51458-16-3 CAPLUS
Benzenepropanoic acid, α-[2-(ethoxycarbonyl)phenyl]-3-hydroxy-4methoxy-, ethyl ester (CA INDEX NAME)

L4 ANSWER 121 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN

N 1973:515413 CAPLUS

N 79:115413

CAPLUS ONEF 79:18743a, 18746a

TI Reactions of the 2-(1H)-pyridinones prepared from 4,4-dimethoxychalcone and anisal acetone

AU Sammour, A.; Fahmy, A. Farouk; Abd El-Rahman, S.; Akhnookh, Y.; Abd Elmoez, M. S.

CS Fac. Sci., Ain Shams Univ., Cairo, Egypt

SU United Arab Republic Journal of Chemistry (1971), 14(6), 581-98

CODEN: UAJCAZ; ISSN: 0372-3704

U Journal

LA English

CF For diagram(s), see printed CA Issue.

ROCCH:CHCGH4OMe-p undervent cycloaddn. with NCCH2CC2Et to give the pyridines I (R = Me, p-MeOCGH4) and the nicotinoates II (R = Me, p-MeOCGH4). MeCOCH:CHCGH4OMe-p and NCCH2CN gave the nicotinate III. I was treated with Grignard reagents, PCC1, and its potassium salt alkylated; e.g. 1 (R = Me) and PhNgbr gave the pyridone IV.

TS 0548-86-2P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RN 50548-86-2C APLUS

CN Benzenepentanoic acid, α-(4-chlorophenyl)-4-methoxy-β-(4-methoxyphenyl)-8-oxo-, methyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 122 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

L4 ANSWER 122 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1973:111801 CAPLUS
N 78:17963a, 17966a
T1 Oxidative carbon-carbon coupling. III. Oxidative polymerization of bifunctional arylcyanoacetic esters
AU De Jongh, H. A. P.: De Jonge, C. R. H. I.: Sinnige, H. J. H.: Magre, E. P.: Mijs, V. J.
CS Corp. Res. Dep., Akzo Res. Lab., Arnhem, Neth.
SJ Journal of Polymer Science, Polymer Chemistry Edition (1973), 11(2), 345-52
CODEN: JPLCAT: ISSN: 0449-296X
DT Journal
LE English
AB Bifunctional arylcyanoacetic esters were oxidatively coupled to give high mol. weight, colorless, amorphous polymers, soluble in common organic solvents.
Brittle films were obtained by casting or compression molding. Thermal stability of the polymer was poor due to the weak C-C bond formed by oxidative coupling. Radical dissociation-recombination of this bond resulted
in meso-dl equilibration, lowering the glass transition temperature of the polymers.

IT 41072-40-6 41072-41-7
RE: PRP (Properties)
(solution and thermal properties of)
RN 41072-40-6 CAPLUS
CN Polyloxy[2,3-dicyano-2,3-bis(4-methylphenyl)-1,4-dioxo-1,4-butanediyl)oxymethylene-1,4-phenylenemethylene) (9CI) (CA INDEX NAME)

RN 41072-41-7 CAPLUS
Poly[oxy[2,3-dicyano-2,3-bis(4-methylphenyl)-1,4-dioxo-1,4-butanediyl]oxymethylene-1,4-cyclohexanediylmethylene] (9CI) (CA INDEX NAME)

L4 ANSWER 123 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN AN 1972:552898 CAPLUS DN 77:152898 OREF 77:25147a,25150a ARAdical-initiated chemical reactions Akzo N. V. Neth. Appl., 8 pp. CODEN: NAXXAN DT Patent LA Dutch FAN.CNT 1 APPLICATION NO. PATENT NO. KIND DATE DATE 19720725 NL 7205982 NL 1972-5982 19720503 Three I and five II were used as radical polymerization initiators for AB Three I and five II were used as radical polymerical and strong styrene
[100-42-5] or Me methacrylate (III) [80-62-6] at 80-120.deg.; 24-98t yields were obtained. In addition II [RI = p-xylylene, R2 = Me, Y = O, n = 190) (IV) was a stabilizer for III <40.deg.. In an example, 25 ml styrene and 56.8 mg IV was kept 2 hr at 120.deg. to give 56 polystyrene [9003-53-6] as compared to 34t for tert-Bu2O2 initiator. The I had R = Me, Bu, or n-decyl with m = 40-60; other II had RI 1,4-dimethylenecyclohewane, cyclohexylidene, or 2,2,4,4-tercamethylcyclohutylene; R2 = Me, or tert-octyl; Y = O or MH; and n = 85-190. 85-190. 38807-91-9 41072-40-6 41072-41-7 IT 38807-91-9 41072-40-6 41072-41-7
RI: CAT (Catalyst use); USES (USes)
 (catalysts, for polymerization of styrene)
3807-91-9 CAPLUS
Poly[1,4-phenylene[1,2-bis (butoxycarbonyl)-1,2-dicyano-1,2-ethanediyl]],
a-(1-cyano-2-methoxy-2-oxoethyl)-a-[4-(1-cyano-2-methoxy-2-oxoethyl)],
oxoethyl)phenyl)- (9C1) (CA INDEX NAME)

RN 41072-40-6 CAPLUS
CN Poly[oxy[2,3-dicyano-2,3-bis(4-methylphenyl)-1,4-dioxo-1,4-butanediyl]oxymethylene-1,4-phenylenemethylene] (9CI) (CA INDEX NAME)

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ANSWER 123 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

41072-41-7 CAPLUS
Poly[oxy[2,3-dicyano-2,3-bis(4-methylphenyl)-1,4-dioxo-1,4-butanediyl]oxymethylene-1,4-cyclohexanediylmethylene] (9CI) (CA INDEX NAME)

L4 ANSWER 124 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) Relative stereochemistry.

30698-39-6 CAPLUS Butamedicio acid, 2.3-bis(4-chlorophenyl)-2.3-dicyano-, dimethyl ester, (R\*,5\*)- [9C1] (CA INDEX NAME)

Relative stereochemistry.

30698-40-9 CAPLUS
Butanedioic acid, 2,3-bis(4-chlorophenyl)-2,3-dicyano-, dimethyl ester, [R\*,R\*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

34404-72-3 CAPLUS 1,1,2,2-Ethanetetracarboxylic acid, 1,2-bis(4-methylphenyl)-, tetramethyl ester (9CI) (CA INDEX NAME)

ANSWER 124 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN N 1972:502330 CAPLUS 77:102330 OREF 77:16876, 16877a TI Radical initiation of vinyl polymerization by //:102307
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//:102307 ΑU peroxides and affected by the  $\alpha$ - and ring-substituents and stereochemistry. The meso- $\alpha$ , dicyanodibenzyls  $\alpha$ ,  $\alpha$  disubstituted with ester groups gave a 2.5-3.5 fold faster polymerization than their DL-isomers.
The dissociation rate consts., determined from NMR line widths, indicated OL-isomers.

The dissociation rate consts., determined from NMM line victor.

The dissociation rate consts., determined from NMM line victor.

a.a'-dicyanodibenzyls a.a'-disubstituted with
ester groups were good initiators while those with Ph and nitrile groups
were inefficient. Initiation and termination mechanisms based on
1, 2-addition of the dibenzyl catalysts to styrene are given.

IT 30698-37-4 30698-38-5 30698-39-6
30698-40-9 34604-72-3 34404-73-4
34405-36-2 34405-37-3 37760-82-0
37761-19-6 37761-20-9 37761-27-0

RL: CAT (Catalyst use): USES (Uses)
(catalysts, for polymerization of vinyl compds.)

RN 30698-37-4 CAPLUS

CR Butanedicic acid, 2,3-dicyano-2,3-bis(4-methylphenyl)-, dimethyl ester,
(R\*,S\*)- (9CI) (CA INDEX NAME)

30698-38-5 CAPLUS Butanedioic acid, 2,3-dicyano-2,3-bis(4-methylphenyl)-, dimethyl ester, (R\*,R\*)- (9CI) (CA INDEX NAME)

ANSWER 124 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

34404-73-4 CAPLUS 1,1,2,2-Ethanetetracarboxylic acid, 1,2-bis(4-chlorophenyl)-, tetramethyl ester (9C1) (CA INDEX NAME)

34405-36-2 CAPLUS Butanedioic acid, 2,3-dicyano-2,3-bis(2-methylphenyl)-, dimethyl ester,  $(R^*,R^*)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

34405-37-3 CAPLUS Butanedioic acid, 2,3-ester, (R\*,R\*)- (9CI) -2,3-dicyano-2,3-bis(2,4-dimethylphenyl)-, dimethyl 9Cl) (CA INDEX NAME)

ANSWER 124 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

1

37760-82-0 CAPLUS Butanedioic acid, 2,3-bis(2-chlorophenyl)-2,3-dicyano-, dimethyl ester, (R.R.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

37761-19-6 CAPLUS Butanedioic acid, 2,3-dicyano-2,3-bis(2-methylphenyl)-, dimethyl ester, (R\*,S\*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

37761-20-9 CAPLUS Butanedioic acid, 2,3-bis(3-chlorophenyl)-2,3-dicyano-, dimethyl ester, (R\*,S\*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L4 ANSWER 125 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1972:447849 CAPLUS
N 77:47849 OREF 77:7922h,7923a
T1 Oxidative carbon-carbon coupling. II. Effect of ring substituents on the oxidative carbon-carbon coupling of arylmalonic esters, arylmalodinitriles, and arylcyanoacetic esters
AU De Jongh, H. A. F.; De Jonge, C. R. H. I.; Sinnige, H. J. M.; De Klein, W. J.; Kluysmans, W. G. B.; Mijs, W. J.; Van den Hoek, W. J.; Smidt, J.
CS Corp. Res. Dep., Akzo Res. Lab., Arnhem, Neth.
SO Journal of Organic Chemistry (1972), 37(12), 1960-6
CODEN: JOCEAH; ISSN: 0022-3263
DJ Journal
LA English
AB Arylmalonic esters and arylmalonodinitriles can be coupled oxidatively to the corresponding bibenzyls. Good yields of dimers are obtained when a para substituent (Me, Cl) is introduced, which inhibits the formation of higher oligomers through benzylic C-para C coupling. Substitution at both ortho positions and the para position (Me) in phenylcyanoacetic esters completely inhibits C-C coupling by steric crowding. Keteneimines are formed instead by C-N coupling. Substitution at one ortho position (Me) partially gives the usual C-C coupling together with benzylic C-para C coupling (Neteneimines formation) in case of a free para-position and C-N coupling (keteneimine formation) in case of a free para-position and c-N coupling (keteneimine formation) in case of a free para-position confirmed by ESR anal. Prom NNR line width measurements kinetic parameters for the dissociation reaction are obtained.

RI: PRP (Properties)
(ESR of)
NN 39514-80-2 CAPUUS
CN Butanedioic acid. 2.3-dicyano-2.3-bis(2.4.6-trimethylphenyl)-, dimethyl ester (9CI) (CA INDEX NAME)

30698-38-5P 34404-72-3P 34404-73-4P 34405-36-2P 34405-37-3P RL: SPN (Synthetic preparation): PREP (Preparation) (preparation of) 30698-38-5 CAPLUS Butanedioic acid, 2, 3-dicyano-2, 3-bis(4-methylphenyl)-, dimethyl ester, (R\*,R\*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L4 ANSWER 124 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

37761-21-0 CAPLUS Butanedioic acid, 2,3-bis(2-chlorophenyl)-2,3-dicyano-, dimethyl ester, (R.5')- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L4 ANSWER 125 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN

34404-72-3 CAPLUS
1,1,2,2-Ethanetetracarboxylic acid, 1,2-bis(4-methylphenyl)-, tetramethyl ester (9CI) (CA INDEX NAME)

34404-73-4 CAPLUS 1,1,2,2-Ethanetetracarboxylic acid, 1,2-bis(4-chlorophenyl)-, tetramethyl ester (9C1) (CA INDEX NAME)

34405-36-2 CAPLUS Butanedioic acid, 2,3-dicyano-2,3-bis(2-methylphenyl)-, dimethyl ester, (R.R.)- (9C1) (CA INDEX NAME)

ANSWER 125 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

34405-37-3 CAPLUS
Butanedioic acid, 2,3-dicyano-2,3-bis(2,4-dimethylphenyl)-, dimethyl ester, (R\*,R\*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L4 ANSWER 126 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

L4 ANSWER 126 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1972:127800 CAPLUS
DN 76:127800
CREF 76:20691a, 20694a
TI Methyl 1,2-diphenylethanetetracarboxylates as initiators for polymerization of styrene
IN De Jongh, Hendrik A. P.; De Jonge, Cornelis R. H. I.
AXZO G.m.b.H.
SO Ger. Offen., 14 pp.
CODEN: GWXEX
DT Patent
LA German
FAN.CNT I
PATENT NO. KIND DATE APPLICATION NO. DATE

DATE
19720120
19800703
19810430
19720105
19731107
19711116
19750722
19700703
19710702
2tetracarb DE 2132740 A 19720120 DE 1971-2132740 19710701 DE 2132740 B2 19800703 DE 2132740 G3 19810430 NL 7009925 A 19720105 NL 1970-9925 19700703 GB 1336675 A 19731107 GB 1971-30874 19710701 BE 769414 A1 19711116 BE 1971-105397 19710702 US 3896099 A 19750722 US 1973-401604 19730928 US 1971-159949 A2 19710702 Tetra-Me 1,2-bis [p-chlorophenyl] ethanetetracarboxylate [34404-71-2], tetra-Me 1,2-bis [p-chlorophenyl] ethanetetracarboxylate [34404-73-4], or tetra-Me 1,2-bis [p-chlorophenyl] ethanetetracarboxylate [1] (34404-72-3], prepared by oxidative coupling of the corresponding di-Me arylmalonates with KMnO4 or K3Fe(CN)6, were used as radical initiators for the merization PRAI

with NMnO4 or K3Fe(CN)6, were used as radical initiators for the
polymerization
of styrene and, in contrast to peroxides or azodinitriles, did not cause
the formation of gaseous products. Thus, 100 ml styrene and 250 mg I were
heated 2 hr at 120.deg, to give 78% polystyrene [9003-53-6] as compared to
34% for tett-Bu peroxide.
IT 34404-72-3 34404-73-4
RL: CAT (Catalystuse); USES (Uses)
(catalysts, for polymerization of styrene)
RN 34404-72-3 CAPLUS
CN 1,1.2.2-Ethanetetracarboxylic acid, 1,2-bis(4-methylphenyl)-, tetramethyl
ester (9CI) (CA INDEX NAME)

34404-73-4 CAPLUS
1,1,2,2-Ethanetetracarboxylic acid, 1,2-bis(4-chlorophenyl)-, tetramethyl ester (9C1) (CA INDEX NAME)

L4 ANSWER 127 OF 146 CAPLUS COPYRIGHT 2007 ACS ON STN
AN 1972:113055 CAPLUS
DN 76:113055
OREF 76:118253a, 18256a
TI Anxiolytic phenyl-2-pyrrolidinene
IN Strubbe, Josef Linz, Rame
PA UCB Union Chiminene
So Ger. Offer

76:18:533,18:508
Anxiolytic phenyl-2-pyrrolidinones
Strubbe, Josef: Linz, Raymond
UCB Union Chimique-Chemische Bedrijven S. A.
Gec. Offen., 32 pp.
CODEN: GWXKEX

CODEN: DT Patent LA German FAN.CNT 1

	PATENT NO.		DATE	APPLICATION NO.	DATE
				4004 0104404	19710722
PΙ	DE 2136571	A	19720127	DE 1971-2136571	19/10/22
	DE 2136571	C2	19820325		
	GB 1350582	A	19740418	GB 1970-35948	19700724
	IL 37147	A	19740630	IL 1971-37147	
	NL 7109930	λ.	19720126	NL 1971-9930	
	FR 2100946	A5	19720324	FR 1971-26784	19710720
	FR 2100946	B1	19750606		
	HU 162344	В	19730129	HU 1971-UI178	
	ES 393496	A1	19730816	ES 1971-393496	
	RO 61127	A1	19761115	RO 1971-67732	19710721
	CS 174822	B2	19770429	CS 1971-5382	19710721
		B2	19770429	CS 1975-6089	19710721
	DK 135584	В	19770523	DK 1971-3580	19710721
	FI 55184	В	19790228	FI 1971-2068	19710721
	FI 55184	С	19790611		
	RO 71354	A1	19820226	RO 1971-81864	19710721
	BE 770308	A1	19720124	BE 1971-3254	19710722
	CA 954870	A1	19740917	CA 1971-118906	19710722
	IN 132195	A1	19750802	IN 1971-132195	19710722
	JP 54017734	В	19790702	JP 1971-54902	
	ZA 7104911	A	19720426	ZA 1971-4911	19710723
	AT 304530	В	19730110	AT 1971-6430	19710723
	AU 7131575	A	19730125	AU 1971-31575	19710723
	CH 537921	A	19730731	CH 1972-10160	19710723
	CH 538474	A	19730815	CH 1971-10857	19710723
	AT 310150	В	19730925	AT 1972-1805	19710723
	SU 479293	A3	19750730	SU 1971-1891416	19710723
	SE 379347	В	19751006	SE 1971-9515	19710723
	SU 488410	A.3	19751015	SU 1971-1689301	19710723
	PL 82184	В1	19751031	PL 1971-149583	19710723
	US 3956314	λ	19760511	US 1973-417528	19731120
PRAI	GB 1970-35948	A	19700724		
	US 1971-165342	AZ	19710722		
GI	For diagram(s), s				

US 1971-165342 A2 19710722
For diagrams(s), see printed CA Issue.
Title compds. [I, R = H, alkyl, PhCH2, propynyl, allyl, or cyclopentyl: R1 = H, alkyl, allyl, or (substituted) phenyl: R2 = H or monosubstituted phenyl: R3 = H, Et, Ph, or 2,4-Me2CGH3] were prepared by several methods: cyclization of 4-aminobutyic acids, decarboxylation of 3-carboxyl-R1-2-pyrolidinones, or known reactions of phenyl-pyrrolidinones gave I (R = H) which reacted with NaH and RI to give 1-substituted I. Thus, p-ClcGH4CH(CNCHPHCOZEt in EtOH was hydrogenated over Raney Ni 15 hr at 90-5° and 100 atm to give .apprx.50% cis-I (R = R3 = H, R1 = Ph, R2 = 4+p-ClcGH4) (II) and the trans isomer separated by crystallization Similarly prepared were .apprx.45 I, e.g. (R-R3 given): Me,
H, 2,4-Me2C6-H3] (III): H, allyl, 3-p-MeCGH4, H; hexyl, Ph, 4-p-ClCGH4, H. Anxiolytic effects were caused by min. doses of 0.0024 mole II/kg rat or

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ANSWER 127 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Co 0.10 mole III/kg rat. 16224-82-59 36263-00-0P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of) 36224-82-5 CAPLUS Benzenepropanoic acid, 4-chloro-a-(4-chlorophenyl)-\$-cyano-, ethyl ester (CA INDEX NAME)

(Continued)

(Continued)

36263-00-0 CAPLUS

Benzenepropanoic acid, 4-chloro-α-(2-chlorophenyl)-β-cyano-, ethyl ester (CA INDEX NAME)

ANSWER 128 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN

30698-40-9 CAPLUS
Butanedioic acid, 2,3-bis(4-chlorophenyl)-2,3-dicyano-, dimethyl ester, (R\*,R\*)- (9CI) (CA INDEX NAME)

#### Relative stereochemistry.

30698-37-4
RL: PRP (Properties): RCT (Reactant): RACT (Reactant or reagent)
(rearrangement of, kinetics of)
30698-37-4
CAPLUS
Butanedioic acid, 2,3-dicyano-2,3-bis(4-methylphenyl)-, dimethyl ester,
(R\*,5\*)- (9CI) (CA INDEX NAME)

#### Relative stereochemistry.

ANSWER 128 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1971:551041 CAPLUS
DN 75:151041
OXIdative carbon-carbon coupling. I. Oxidative coupling of
a-substituted benzylcyanides
AU De Jongh, H. A. P.; De Jonge, C. R. H. I.; Mijs, W. J.
CS Corp. Res. Dep., Akzo Res. Lab., Arnhem, Neth.
SO Journal of Organic Chemistry (1971), 36(21), 3160-8
CODEN: JOCEAN: ISSN: 0022-3263
J Journal
LA English
GF for diagram(s), see printed CA Issue.
AB OXidative dimerization of benzylcyanides a-substituted with an
ester, acyl, or amide group, with a Cu-amine-O system or with other
oxidants gave the corresponding 2,3-diphénylsuccinomitriles as a mixture of
diastereoisomers in high yields. Configurational assignments are made for
dl- and meso-I on the basis of cyclization reactions to give mono or
bicyclic succinimides II and III. Thermal equilibration of the dl and
meso diastereoisomers takes place in various solvents at 80-150'
via radical dissociation-recombination along the central C-C bond. For

via radical dissociation-recombination along the central C-C bond. ror dimers

(I (R-H, Me) the equilibrium constant K (dl/meso) is 13-16. For the meso - dl conversion of I (R-H, Me), AH\* is 22-23 kcal/mole and AS\* is -11 to -12 entropy units. Thermal treatment of the para unsubstituted diester I (R-H) at 130-170\* gives redistribution to the monomer PhCH(CN)CO2Me (IV) and oligomers (tri-to pentamers). Similarly, the oxidative coupling of the para unsubstituted benzylcyanides IV, PhCH(CN)Ac, and a-{piperidinocarbonyl}benzylcyanide gave rise to various amounts of oligomers. Both oligomerization reactions are impeded by introduction of a para substituent.

1 30698-38-5P 30698-39-6P 30698-40-9P

RL: SPN (Synthetic preparation): PREP (Preparation)
(preparation of)
RN 30698-38-5 CAPLUS

CN Butanedioic acid, 2,3-dicyano-2,3-bis(4-methylphenyl)-, dimethyl ester, (R\*,R\*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

30698-39-6 CAPLUS

Butanedioic acid, 2,3-bis(4-chlorophenyl)-2,3-dicyano-, dimethyl ester, (R\*,S\*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

OREF TI

ANSWER 129 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN
1971:510166 CAPLUS
75:110166
75:110166
75:17395a,17398a
Isoquinoline-type heterocycles from β-amino acids. II.
Stereospecific syntheses of (+-)-6,7-dialkoxy-3-aryl-4-(methoxycarbonyl)1,2,3,4-tetrahydroisoquinolines and their derivatives
Haimova, Marietta A.; Spassov, Stefan L.; Novkova, Snezana I.; Palamareva,
Mariana D.; Kurtev, Bogdan J.
Fac. Chem. Univ. Sofia, Sofia, Bulg.
Chemische Berichte (1971), 104(8), 2601-10
CODEN: CHEEAM; ISSN: 0009-2940
JOURNAI
German
For diagram(s), see printed CA Issue. AU

CS SO

German
For diagram(s), see printed CA Issue.
Me (t)-3-amino-2,3-diarylpropionates gave under the conditions of the
Pictet-Spengler reaction by cyclization stereospecifically in both the
erythro and threo series 6,7-dialkowy-3-aryl-4-(methoxycarbonyl)-1,2,3,4tetrahydroisoquinolines (I). LiAlH4 reduction of I gave the corresponding
4-hydroxymethyl derivs. From the NMR data reported, the conformations of
the compds. are evaluated.
33386-60-D 33386-65-IP 33386-66-2P
33482-67-6P

33482-67-6P
RL: SPN (Synthetic preparation), PREP (Preparation)
(preparation of)
3386-64-0 CAPLUS
β-Alanine, 2-(2-bromo-4,5-dimethoxyphenyl)-3-[2-bromo-4,5-(methylenedioxy)phenyl]-N-formyl-, methyl ester, erythro-(±)- (8CI)
(CA INDEX NAME)

Relative stereochemistry.

33386-65-1 CAPLUS \$\text{B-Alanine}\$, 2-(2-bromo-4,5-dimethoxyphenyl)-3-{2-bromo-4,5-(methylenedioxy)phenyl}-, methyl ester, erythro-(\$\text{2}\$)- (\$\text{RCI}\$) (CA INDEX NAME)

33386-66-2 CAPLUS B-Alanine, 2-(2-bcomo-4,5-dimethoxyphenyl)-3-[2-bromo-4,5-(methylenedioxy)phenyl]-, methyl ester, hydrochloride, erythro-(±)-(8C1) (CA INDEX NAME)

Relative stereochemistry.

• HC1

33482-67-6 CAPLUS B-Alanine, 2-(2-bromo-4,5-dimethoxyphenyl)-3-[2-bromo-4,5-(methylenedioxy)phenyl]-N,N-dimethyl-, methyl ester, erythro-(±)- (8CI) (CA INDEX NAME)

Relative stereochemistry.

L4 ANSWER 130 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1971:88362 CAPLUS
DN 74:88362
OREF 74:14349a,14352a
OREF 74:14349a,14352a
T1 \* 1,2-Diphenyl-1,2-dicyano-1,2-bis[alkyl (or aryl or amino)peroxy (or oxy)
carbonyl]ethanes as polymerization initiators
N De Jongh, Hendrik A.; De Jonge, Cornelis R. H. I.
PA AXZO N. V.
SO Ger. Offen., 18 pp.
COODEN: GWXXEX
DT Patent
LA German
FAN.CNI 1
PATENT 10

LWN	.CNI I						
PATENT NO.		KIND	DATE	APPLICATION NO.	- DATE		
	***						
PΙ	DE 2033910	A	19710121	DE 1970-2033910	19700708		
	DE 2033910	B2	19810219				
	DE 2033910	C3	19811217				
	NL 6910428	A	19710112	NL 1969-10428	19690708		
	NL 161425	С	19800215				
	NL 161425	В	19790917				
	US 3726837	A	19730410	US 1970-52073	19700702		
	GB 1270784	A	19720412	GB 1970-1270784	19700707		
	BE 753154	A	19701216	BE 1970-753154	19700708		
	FR 2054344	A5	19710416	FR 1970-25339	19700708		
	AT 300346	В	19720725	AT 1970-6212	19700708		
	JP 49045151	В	19741202	JP 1970-59171	19700708		
	SE 371011	В	19741202	SE 1970-9465	19700708		
PRA	T NI. 1969-10428	A	19690708				

SE 371811 B 1974/202 SE 1970-9465 19700708
PRAI NL 1969-10428 A 19690708
AB The reaction-specific, fairly heat-stable compds. of the formula NC(p-R C6H4)[R1(0) noC]CC(C0(0) nnl] (C6H4-p)CN (1), where R = H, Me, Cl. NO2, or OMe: R1 - Me, Et. Ph, NHZ, NEMe, or pipe ridino, n = 0-1, oxidation resistant, of relatively high activity at lower temps., inactive at room temperature, and which do not form gaseous products during radical formation are useful as radical initiators for polymerization, e.g., of styrene (II), AcOCH:CHZ, CHZ:CHCN, or CHZ:CMCOCMe, or the hardening, e.g., of the unsatd, polyester resin Lupodal P-6. I are prepared by treating the corresponding NC(p-RC6H4)CH(CO(0)nR1) with O in the presence of CuCl and MeZNCHZCHZNNe2.
IT 31249-03-3 31249-04-4 31249-05-5
RL: CAT (Catalyst use): USES (Uses)
(catalysts, for polymerization of vinyl compds.)
RN 31249-03-3 CAUPU polymerization of vinyl compds.)
RN 31249-03-3 CAUPU polymerization of vinyl compds.)
CN Butanedioic acid, 2,3-dicysno-2,3-bis(4-methylphenyl)-, dimethyl ester (9C1) (CA INDEX NAME)

31249-04-4 CAPLUS Succinic acid, 2,3-dicyano-2,3-di-p-tolyl-, didodecyl ester (8CI) (CA INDEX NAME)

ANSWER 129 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

ANSWER 130 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

31249-05-5 CAPLUS . Succinic acid, 2,3-bis(p-chlorophenyl)-2,3-dicyano-, dimethyl ester (8CI) (CA INDEX NAME)

ANSWER 131 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1969:491021 CAPLUS 71:91021 71:16914h,16915a Non-volatile a-branched chain fatty acid derivatives. IV. Addition of aryl esters to long chain olefins Bilyk, A.; Eisner, A.; Maerker, G. Eastern Util. Res. and Develop. Div., Agr. Res. Serv., Philadelphia, PA, JOHN 10 of the American Oil Chemists' Society (1969), 46(9), 469-72 CODEN: JAOCA7: ISSN: 0003-021X 50 DT LA AB Journal English
The di-tert-butyl peroxide initiated free radical addition of Me phenylacetate (1), Me p-tolylacetate, and Me p-methoxyphenylacetate to 1-decene gives two types of products. In addition to the expected a-branched esters, dehydrodimer (both meso and dl) esters were also obtained. The highest yield of a-branched ester was obtained from I. Higher yields of the dehydrodimer esters were obtained from the substituted phenyl esters. Attempts to add Me p-nitrophenylacetate to 1-decene were not successful and no evidence for the formation of a dehydrodimer product was observed.

25169-83-9P 25169-84-0P
RL: SPN (Synthetic preparation): PREP (Preparation) 25|157-87-97 25|057-84-07 RE: SPN (Synthetic preparation): PREP (Preparation) (preparation of) 25|05-83-97 CAPLUS Butanedioic acid, 2,3-bis(4-methylphenyl)-, dimethyl ester, (R\*,S\*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

25169-84-0 CAPLUS Butanedioic acid, 2,3-bis(4-methylphenyl)-, dimethyl ester, (R\*,R\*)- (9CI) (CA INDEX NAME)

Relative stereochemistry

ANSWER 132 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN
1967:481889 CAPLUS
67:81889 F 67:51816a, 15418a
Reaction of potassium cyanide with p-phenylsulfonylbenzyl bromide
Lotspeich, F. J.
West Virginia Univ. Med. Center, Morgantown, WV, USA
Journal of Organic Chemistry (1967), 32(4), 1274-7
CODEN: JOCEAH; ISSN: 0022-3263
Journal
English
p-Phenylsulfonylbenzyl bromide (I) is treated with KCN to give
a, a-bis(p-phenylsulfonylbenzyl)-p-phenylsulfonylbenzyl
cyanide. I treated with NaI in Me2CO gives p-PhSO2CGH4CH2I. Also prepared,
from p-PhSO2CGH4COCI and CH2N2, is p-PhSO2CGH4COCH2N2 which is treated
with Ag2D to give p-PhSO2CGH4COCH2N2 which is treated
with Ag2D to give p-PhSO2CGH4COCH2N2 which is treated
FRL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
7705-67-17 CAPLUS
Propionic acid, 2,3-bis[p-(phenylsulfonyl)phenyl]-, methyl ester (8CI)
(CA INDEX NAME)

L4 AN DN OREF TI bb:13265a,13266a
Infrared and ultraviolet spectra of organomercury compounds. II.
Ultraviolet spectra of ethyl a-bromomercuriarylacetates
Artamkina, G. A.: Beletskaya, I. P.: Pentin, Yu. A.: Reutov, O. A.
State Univ., Moscow, USSR
Zhurnal Organicheskoi Khimii (1966), 2(8), 1329-34
CODEN: 2ORKAE: ISSN: 0514-7492
Journal Journal Russian of CA 63, 13024f. Uv spectra were reported for XCGH4CH(HgBr)CO2Et where X e H. Me, I, NO2, Et, iso-Pr, tert-Bu, F, Cl, and Br in the para position, Me or Br in the ortho position, and Br or Me in the meta position. These esters had 2 characteristic bands at 208-217 and 252-260 mg. A comparison with XCGH4CH2CO2Et and XCGH4CHBCO2Et was made: the substituents on the CH2 bridge affect the spectra more significantly than do the ring substituents.

15098-17-6 RELUS (spectrum (uv) of) 15098-17-6 CAPLUS (Succinic acid, 2,3-di-p-tolyl-, diethyl ester (7CI, 8CI) (CA INDEX NAME) ΙT

ANSWER 133 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1967:70525 CAPLUS 66:70525 66:13263a,13266a

L4 ANSWER 134 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN AN 1966:429366 CAPLUS DN 65:29366 OREF 65:5434e-f TI Flavanoids. II. Stereochemistry of isoaurones AU Marathe, K. G.: Byrne, M. J.; Vidwans, R. N. Univ. Poona, India 65:29366

F 65:5434e-f

Flavanoids. II. Stereochemistry of isoaurones

Marathe, K. G.: Byrne, M. J.: Vidwans, R. N.
Univ. Poona, India

Tetrahedron (1966), 22(6), 1789-95

CODEN: TETRAB: ISSN: 0040-4020

Journal

English

cf. CA S4, 3402a. Isoaurones (anhydrolactones of 2-hydroxy-a
benzylmandelic acids), trimethylanhydrohazeyl lactone and its

5-methyl-4'-methoxy analog are shown to be trans-stilbene derivs, and are

isomerized to the cis compds. by pyridine. The stereochemistry has been

established by a stereoselective synthesis of the derived

cis-stilbene-a-carboxylic acid and confirmed by uv and N.M.R.

studies. A mechanism for isomerization has been suggested.

6581-70-0 G600-69-7

(Derived from data in the 7th Collective Formula Index (1962-1966))

6581-70-0 CAPLUS

Mandelic acid, 2-methoxy-a-(p-methoxybenzyl)-5-methyl-, ethyl ester

(7CI, 8CI) (CA INDEX NAME)

6600-69-7 CAPLUS Mandelic acid, 2-ethoxy- $\alpha$ -(p-methoxybenzyl)-5-methyl-, ethyl ester (7CI, 8CI) (CA INDEX NAME)

6581-74-4P, Lactic acid, 3-(p-methoxyphenyl)-2-(6-methoxy-m-tolyl)-, methyl ester
RL: PREP (Preparation)
(preparation of)
6581-74-4 CAPLUS
Mandelic acid, 2-methoxy-α-(p-methoxybenzyl)-5-methyl-, methyl ester
(8CI) (CA INDEX NAME)

L4 ANSWER 135 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN AN 1966:429365 CAPLUS ON 65:29365 OREF 65:5434a-e
TI Heraclenin from Hippomarathrum microcarpum AU Kerimov, S. Sh. CS. V. L. Komarov Botan. Inst., Leningrad SD Zhurnal Prikladnoi Khimii (Santana)

bs: 93:43-e
Heraclenin from Hippomarathrum microcarpum
Kerimov, S. Sh.
V. L. Komancov Botan. Inst., Leningrad
Zhurnal Prikladnoi Khimii (Sankt-Peterburg, Russian Federation) (1966),
39(3), 660-4
CODEN: ZPXHAB; ISSN: 0044-4618
Journal
Russian
For diagram(a), see printed CA Laque.

LA Russian

(I For diagram(s), see printed CA Issue.

AB Heraclenin (1), m. 107-8°, [e]220 25.5° (c 2.51,
pyridine), was extracted from H. microcarpum (II). II was extracted with

CHCl3 to

give 200 g. extract, which was dissolved in a min. quantity of CHCl3 and
chromatographed on a column containing neutral A1203. The substances were
eluted from the column with petroleum ether, b. 40-60°, with a
petroleum ether-CHCl3 (4: 1) mixture, or with CHCl3 and with MeOH. Elution

with a petroleum ether-CHCl3 mixture gave 2 substances. After evaporation

with a periodom conof the
eluate, the residue was dissolved in 4:1 EtOH-CHCl3 to give
hydroxypeicedanine. The mother liquor gave crystals which were recrystd.
from 4:1 alc.-petroleum ether to give I, m. 107-8\*, [a]22D
25.5\* (c 2.51, pyridine), Rf 0.31. I (2 g.) added to a hot solution
of 0.3 g. (CO2H)2 in 20 ml. H2O, the mixture refluxed 45 min., cooled,

ted with water, and extracted with CHCl3, the extract evaporated, the residue chromatographed on an inactive Al203 column, and eluted with CHCl3 and EtOH, and the EtOH eluate evaporated to give I hydrate, m. 114-15', v. 3400 cm.-1, Amax 220, 250, 362, 300 ms. I (0.5 g.) was added to 225 ml. 108 H2SO4, and the mixture boiled 15 min., filtered hot, and cooled to give isoheraclenin, m. 132.5-4.5' (EtOH), Amaximum 220, 250, 262, 300 ms. I (0.2 g.) was dissolved in 10 ml. AcOH, 5 drops concentrated H2SO4 added, the mixture heated on a water bath

left overnight, and diluted with ice water, a yellow product separated, chromatographed on inactive Al203, and eluted with 20:1 Me2COAcOH, the eluate evaporated and the residue crystallized to give manthotoxol (III), m. 240-1' [ECHD], Amaximum 224, 250, 268, 308 pm, Rf 0.73. III [0.2 g.] was dissolved in 6 ml. MeOH, 0.1NKOH added to weak alkaline

reaction,
0.3 g. MeI gradually added, the mixture boiled 1.5 hrs., MeOH distilled, and
the residue crystallized to give \*\*anthotoxin, m. 145-6\*, Rf 0.21. The
ir spectrum of I was compared with that of parngenin. I is 1 of the
enantiomers of the racemic compound, parngenin.
IT 6581-70-0 6600-69-7

(Derived from data in the 7th Collective Formula Index (1962-1966)) 6581-70-0 CAPLUS

Mandelic acid, 2-methoxy-q-(p-methoxybenzyl)-5-methyl-, ethyl ester (7CI, 8CI) (CA INDEX NAME)

ANSWER 134 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN

ANSWER 135 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

6600-69-7 CAPLUS Mandelic acid, 2-ethoxy- $\alpha$ -(p-methoxybenzyl)-5-methyl-, ethyl ester (7CI, 8CI) (CA INDEX NAME)

L4 ANSWER 136 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN AN 1964:61005 CAPLUS DN 60:61005 OREF 60:10707a-d

Synthesis of some organomercury salts of the type XC6H4CH(HgBr)CO2Et Beletskaya, I. P.; Artamkina, G. A.; Shevlyagina, E. A.; Reutov, O. A. Zhurnal Obshchei khimii (1964), 34(1), 321-4 CODEN: ZOXHA4; ISSN: 0044-460X

Journal

Unavailable cf. CA 57, 16645e. o-BrC6H4CH2CN refluxed in EtOH-concentrated H2SO4 5 h.

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of. Ca S7, 16645e. o-BrC6H4CH2CN refluxed in EtOH-concentrated H2SO4 5 h.

77% o-BrC6H4CH2CO2Et (I), b7 128°, m. 34.5°. Similarly was prepared the m-isomer, 75%, b2 120-1°, n200 l.5348, d20 l.3810. p-EtC6H4CH2CO2Et, b4 110°, l.4970. l.013, was prepared in 82% yield from the acid and EtOH. I in CC14 was brominated under an incandescent lamp and gave XC6H4CHECO2Et (II) (X = 0-Br), 50%, b) 107°, l.5781, l.7266. Similarly was prepared the m-isomer, 60%, b3 148-9°, l.5781, l.7266. Similarly was prepared the m-isomer, 60%, b3 148-9°, l.5712, l.7010, and II (X = p-O2N), 55%, b4 165°, l.5580, -Et p-ethylmandelate and PBT3 in CHC13 at first with cooling, then 0.5 h. on a steam bath, gave 73% p-EtC6H4CHECO2Et, b4 125°, l.5350, l.3227. Similarly were prepared 60% p-iso-PT analog, b6 142°, l.5260, l.2800, and p-methoxy analog, 65%, b3 150°, l.5500, l.4050. Shaking II with H3 gave 51% p-MecC6H4CH(H9BF)CO2Et (III), m. 70°, 50% o-bromo analog, m. 91°, 40% m-bromo analog, m. 69°, 70% p-Et analog, m. 95°. In case the product precipitated as an oil, indicating the formation of R2Hg, the mixture was treated with H3BT2 to effect conversion to RH3BT. If the preparation of III was cun at 50°-60°, the product was 60% (p-MecC6H4CHCO2Et)2, m. 151°. Similarly was obtained the p-ethylphenyl analog, 15%, m. 125°. The reaction of the p-anisyl member with H3 gave only a tar that was free of H3. A previously reported substance (loc. cit.), m. 145°, was shown to be BrH3CH2CGH4CH2CO2Et, rather than III.
15098-17-6F, Succinic acid, 2,3-di-p-tolyl-, diethyl ester
RL: PREP (Preparation)
(preparation of)
15098-17-6F, Succinic acid, 2,3-di-p-tolyl-, diethyl ester
RL: PREP (Preparation)
(preparation of)
15098-17-6 CAPLUS

Succinic acid, 2,3-bis(p-ethylphenyl)-, diethyl ester (7CI) (CA INDEX NAME)

ANSWER 137 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1963:66251 CAPLUS

58:66251

DN 58:66251

OREF 58:11265g-h, 11266a-h, 11267a-f

TI Reaction of diazomethane with double bonds. I. Direct methylation of trisubstituted tehylenes

AU Alguero, M.: Bosch, J.: Castaner, J.: Castella, J.: Castells, J.: Mestres, R.: Pascual, J.: Serratosa, F.

CS Univ. Barcelona, Spain

OTECTARAB: ISSN: 0040-4020

DT Journal TARAB: ISSN: 0040-4020

Journal Unavailable

Unavailable

For diagram(s), see printed CA Issue.

Cf. CA 57, 12455d. Treatment of "phenzylidene-a
carboxybutenolide (I, R = COZH, (R' = H) (4.0 g.) in 15 ml. Et20 at

20° with 2.-2-4 moles CHZN2 in Et20 and the product recrystd. from

Et20 (or Et0Ac) gave 3.8 g. y-benzylidene-a-carbosethoxy
methylbutenolide (II, R = COZHe, R' = H) (IIII), m. 156-8°, µ,

1786, 1726 cm.-1 (CC14), x 202, 227 mµ (s. 14,500, 7180),

also produced (0.3 g.) by treatment of I (R = COZHe, R' = H) (0.3 g.) in

Et20 with 1.2-1.4 moles CHZN2 in Et20. Similarly were prepared II (R, R'

and m.p. given): CN, H, 167-90'; COZHe, Me, m. 154-7';

COZMe, Cl, 175.0-7.5°, COZMe, NO2, 166-72° (decomposition). I (R

R' = H) (0.2 g.) treated with excess CHZN2 in Et20 gave unchanged

starting material. III (7.23 g.) heated 10 hrs. (N atmospheric) in 200 ml.

dioxane and 80 ml. concentrated HCl and the washed (alc., H2O) precipitate

ystd.

From diowane gave 5.22 g. II (R = CO2H, R' = H) (IV), m. 190-2\* (decomposition), v 1757, 1724 cm.-1 (CHCl3), \( \lambda 202, 231, 344 mp \) (= 11,300, 7800, 26,400). IV (196 mg.) and 0.2 ml. concentrated HCl refluxed 13 hrs. in 12 ml. MeOH and treated with EtOAc, the filtered

to 11,000, 150, 20,000, 1 1,100 mg.; and 0.2 ml. Contentrated in 1 solution

vashed with 2N aqueous K2CO3 and H2O, percolated through an Al2O3 column and the eluate evaporated gave III, also obtained by methylation of IV with ethereal CH2N2. The acids II (R = COZI, R\* = Me, Cl), m. 202-10\* (decomposition), \( \text{ 202, 4}, 233, 51 \) mu (e 16,700, 10,130, 37,900), and m. 208-18\* (decomposition), \( \text{ 202, 423, 342-3 mm} \) (e 12,330, 12,500, 32,700), were similarly prepared IV (2.0 g.) heated in vacuo at 250\* and the product distilled at 210\*/18 ms. gave 0.8 g. solid, recrystd: from Et2O to give II (R = R\* = H) (V), m. 101-3\*, v. 1786, 1387 cm.-1 (CC14), \( \text{ 226, 240, 324 mm} \) (e 9150, 7960, 20.490). V (1.0 g.) in 20 ml. 401 HI and 20 ml. AcOH heated 6 hes. at 160\* in a sealed tube and the cooled mixture diluted with H2O, treated with a few drops of aqueous Na2CO3 and the alkaline solution acidified with ZN HC1. The acid solution extracted with Et2O, and the

acidified with 2N HCl, the acid solution extracted with Et2O and the

acidities with an acceptance of the petr. ether gave 0.96 g. PhCH2COCHMeCH2CO2H evaporation recrystd. from petr. ether gave 0.96 g. PhCH2COCHMeCH2CO2H

0.6 g.
4-methyl-2-phenyl-cyclopentane-1,3-dione, n. 181-3\*.
PhCH2COCHMeCOZET (10.0 g.) in 35 ml. C6H6 treated with NaOEt (from 1.15 g.
Na in 15 ml. alc.) and the C6H6 distilled, the mixture refluxed 9 hrs. with

g. BrCH2CO-2Et in 10 ml. C6H6 and acidified with 2N H2SO4, the C6H6 layer washed with 0.5M aqueous NaHCO3 and H2O and distilled in a high vacuum gave

ANSWER 136 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN

ANSWER 137 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) g. oil, b0.1 131-2\* n220 1.4960. This oily PhCHIZCOCME (COZET) CHIZCOZET (8.18 g.)shaken 24 hrs. with 8.18 ml. 104 XOH in dioxane, the mixt. washed with Et20 and acidified with 2N HCL, extd. with Et20 and the residue on evapn. recrystd. from 1:3 Et20-petr. ether gave VI. VI (0.44 g.) and 2.9 g. KOH in 2.5 ml. 804 NZH4 HLZO and 5 HLZO AND 4:9 g. KOH in 2.5 ml. 804 NZH4 HLZO and 5 HLZO AND 4:9 g. KOH in 2.5 ml. 804 NZH4 HLZO and 5 HLZO washed and dried ext. evapd., the residue (0.34 g.) chromatographed in CCHG cover silica gel and eluted with 20: 1 CGHGEZO gave 0.34 g. oily PhCHIZCHZCHMECHZ-COZE, B0.6 210\*; anitide m. 109-111\* p-toluide m. 107-8\*. EtHgBr (from 2.43 g. Ng) in 80 ml. Et20 stirred (N atm.) with dropwise addn. of 11.2 g. PhC.tplbond.CH in 20 ml. dty CGHG and the mixt. refluxed 7 eths. treated dropwise at 20\* with 12.7 g. N-accetylpiperidine (VIa) in 50 ml. dty CGHG and stirred 17 hrs. eth. 21.2 g. PhC.tplbond.CH in 20 ml. dty CGHG and the mixt. refluxed 2 hrs., treated dropwise at 20\* with 12.7 g. N-accetylpiperidine (VIa) in 50 ml. dty CGHG and stirred 17 hrs., extd. stimes vice 100 ml. Et20 and the with 200 GHG and stirred 17 hrs., extd. stimes vice 100 ml. Et20 snd the washed with 20.6 M aq. NABCO3 and HZO, evapd. and the residue distr. gave 1.95 g. VIa, b0.8 G-7-04 and 1.20 g. PhC.tplbond.Chc (VII), b0.8 75-6\* μ. 2208, 169 ml. et 10.2 g. PhC.tplbond.Chc (VII), b0.8 75-6\* μ. 2208, 169 ml. et 10.2 g. PhC.tplbond.Chc (VII), b0.8 75-6\* μ. 2208, 169 ml. et 10.2 g. PhC.tplbond.Chc (VII), b0.8 75-6\* μ. 2208, 169 ml. et 10.2 g. PhC.tplbond.Chc (VII), b0.8 75-6\* μ. 2208, 169 ml. et 10.2 g. PhC.tplbond.Chc (VII), b0.8 75-6\* μ. 2208, 169 ml. et 10.2 g. PhC.tplbond.Chc (VII), b0.8 75-6\* μ. 2208, 169 ml. et 10.2 g. PhC.tplbond.Chc (VII), b0.8 75-6\* μ. 2208, 169 ml. et 10.2 g. PhC.tplbond.Chc (VII), b0.8 75-6\* μ. 2208, 169 ml. et 10.2 g. PhC.tplbond.Chc (VII), b0.8 75-6\* μ. 2208, 169 ml. et 10.2 g. PhC.tplbond.Chc (VII), b0.8 75-6\* μ. 2208, 169 ml

ANSWER 137 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) (C2C14), 0.36 g. V. and 0.10 g. mixt. An atteepted synthesis of 1-methyl-3-phenylpropacyylidenemalonic acid (for further cycliration to a-carboxy-9-methylputenolide) by condensation of VII and HZC (CO2H) 2 gave a neg. result. VII (0.38 g.), 0.67 g. NCCHZCOZH, and 2 ml. AcOH heated (N atm.) 82 hrs. at 100° and dild. with 3 ml. HZO and 3 ml. petr. ether, filtered, and the washed residue recrystd. from CCH6 gave 0.15 g. II (R = CN, R° = H), hydrolyzed (0.10 g.) by heating 3 hrs. at 100° in 2.5 ml. AcOH and 3 ml. 601 HZSO4 to IV. The 9-methylbutenolide structure of the compds. I and II was also established by a study of their hydrogenated derivs. (VIII). IV (200 mg.) in 33 ml. abs. alc. and 2 ml. HZO conty. 75 mg. XCH Hydrogenated at 14°,752 ms. with 33 mg. PtO2 and adsorption of 2.08 moles H, the mixt. treated with 0.27 ml. 2M HCl and the filtered soln. evapd. in vacuo, the residue taken up in 30 ml. HZO, acidified with 2N HCl, extd. with 1:10 CCH31-HZO, and the oily product rubbed with Et2O gave 90 mg. VIII (R = COZH) (IX), m. 123-7°, v 1783, 1721 cm. -1 (CH-C13). The Et2O soln. extd. with an NaHCO3 and the alk. ext. acidified, extd. with Et2O, and the sirupy product chromatographed over silica gel yielded 401 stereoisomeric mixt. of acids. III (2.0 g.) in 75 ml. alc. hydrogenated over 0.1 g. PtO2 and the filtered soln. evapd. gave a colorless, fluid resin VIII (R = COZH), bo.01 140°, refluxed (2.0 g.) vith 2.0 g. XOH in 20 ml. alc. 1 hr. and the cooled mixt. filtered, the K salt taken up in HZO and acidified vith 22N HCl to yield 0.9 g. IX. IX (2.0 g.) heated 30 min. at 140° in vacuo and the residue distd. gave 0.8 g. VIII (R = H) (X), bo.75 130°, v. 17779 cm. -1 V (1.0 g.) in 50 ml. alc. hydrogenated over 60 mg. PrO2 and the filtered soln. evapd. gave a colorless oil, bo.75 130°, vo 17779 cm. -1 V (1.0 g.) in 50 ml. alc. hydrogenated over 60 mg. PrO2 and the residue distd. gave 0.8 g. VIII (R = H) (X), bo.75 130°, vo 17779 cm. -1 V (1.0 g.) in 50 ml

ANSWER 137 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) 98333-22-3 CAPLUS Succinic acid, 2-m-tolyl-3-p-tolyl-, diethyl ester (7CI) (CA INDEX NAME)

98333-28-9 CAPLUS

Succinic ac INDEX NAME) cinic acid, 2-(p-methoxyphenyl)-3-p-tolyl-, diethyl ester (7CI) (CA

ANSWER 137 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) 1509a-17-6 CAPLUS Succinic acid, 2,3-di-p-tolyl-, diethyl ester (7CI, 8CI) (CA INDEX NAME)

97116-28-4 CAPLUS Succinic acid, 2,3-di-o-tolyl-, diethyl ester (6CI, 7CI) (CA INDEX NAME)

97116-29-5 CAPLUS Succinic acid, 2-o-tolyl-3-p-tolyl-, diethyl ester (7CI) (CA INDEX NAME)

98333-21-2 CAPLUS Succinic acid, 2,3-di-m-tolyl-, diethyl ester (7CI) (CA INDEX NAME)

ANSWER 138 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1962:483341 CAPLUS 57:83341

AN 578-3341
OREF 57:16645-h
T Synthesis of some organomercury salts of type XCGH4CH(HgBr)CO2C2H5.II
OREF 57:16645-h
Beletskaya, I. P.: Reutow. O. A.: Artamkina, G. A.
Chunal Obshchei Khimii (1962), 32, 241-4
CODEN: ZOKH44: ISSN: 0044-460X
DJ Journal
LA Unavailable
Unavailable
A cf. CA 55, 21014b. Adding 18 ml. Br to 55 g. p-FCGH4CH2CO2H and 2.8 g. red P in refluxing CHCl3, refluxing until HBr evolution ceased, and adding 23 ml. Br with heating gave after heating with 30 ml. EtOH followed by aqueous

red P in refluxing CHC13, refluxing until HBr evolution ceased, and addi 23 ml. Br with heating gave after heating with 30 ml. EtoH followed by courseling the heating gave after heating with 30 ml. EtoH followed by courseling the heating gave after heating with 30 ml. EtoH followed by treatment, 43h p-FCGH4CHBCO2Et, b) 105-6°, n20D 1.4558, m.

12°, and 22% p-FCGH4CHBCO2Et, b) 120-2°, n20D 1.5190, d20
1.4623. Similarly were prepared: p-BrCGH4CHBCO2Et, 53, b3 130-2°, 1.5578, 1.6600, p-1CGH4CHBCO2Et, 10%, m. 52°, p-ICGH4CHBCO2Et, 25%, m. 29°. The residue from the last substances treated with 130°, and less soluble in Et2O, (p-ICGH4CHBCO2Et) m. 170-1°, also were prepared: 5% 0-MeGGH4CHBCO2Et, b7 132-4°, 1.5397, 1.3721; 53% m-isomer, bt 130-2°, 1.5348, 1.3536; 76% p-Me3CGH4CHBCO2Et, b2 140-2°, 1.5300, 1.2660; 5% p-Me3CGH4CHBCO2Et, b7 152-4°, 1.5590, p-1; ncandescent lamp illumination gave 85% p-FCGH4CHBCO2Et (11), b3 105-6°, 1.5503, p-B nanalog, 76%, b3 130-3°, 1.5503, p-; p-I nanalog, 44%, m. 52°. II shaken 4 hrs. with Hg gave 24% p-FCGH4CH(HgBFLCO2Et, m. 95°. Similarly were prepared: 9% p-Br analog, m. 120-20.5°; p-I analog, 57%, m. 122°; o-MeCGH4CH(HgBFLCO2Et, 75%, m. 94°; p-Me3CGH4CH(HgBFLCO2Et, 75%, m. 94°; p-Me3

94550-49-9 CAPLUS Succinic acid, 2-bromo-2,3-bis(p-iodophenyl)-, diethyl ester (7CI) (CA INDEX NAME)

ANSWER 138 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN

L4 ANSWER 139 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN

114791-94-5 CAPLUS

114 791-94-5 CAPLOS 4H-1-Benzopyran-6-acetic acid, a,5,7-trihydroxy-a-p-hydroxybenzyl-2-(p-methoxyphenyl)-4-oxo-, ethyl ester (6CI) (CA INDEX NAME)

115099-51-9 CAPLUS
4H-1-Benzopyran-6-acetic acid, a,5-dihydroxy-7-methoxy-a-p-methoxybenzyl-2-(p-methoxyphenyl)-4-oxo-, ethyl ester (6CI) (CA INDEX NAME)

L4 ANSWER 139 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1961:17917 CAPLUS
DN 55:17917
OREF 55:3579a-f
T1 The structure of ginkgetin. V. Flavone carboxylic acid
AU Kogure, Akira
CS Osaka City Univ.
SO Nippon Kagaku Zasshi (1959), 80, 1462-6
CODEN: NPRZAZ; ISSN: 0369-5387
DT Journal Nippon Kagaku Zasshi (1959), 80, 1462-6
CODEN: NPKRZA: ISSN: 0369-5387
Journal
Unavailable
A flavonecarboxylic acid. C25H2009 (I), was obtained from ginkgetin (Ia)
by treating with KOH-H2O, which gave the Me ether Me ester (II) with CH2N2
(cf. preceding abstract). II showed pos. FeCi3 reaction, & 2.71,
3.21, 5.8, 6.00 µ, suggesting the existence of still more hydroxy
groups. II heated with Ac2O and AcONa gave the two acetates, C30H2608, m.
139-141', and C32H30011, m. 196-8' II gave the carboxylic
acid Me ether (III), C27H2409, pale yellow, insol. in NaHCO3 solution III
gave C27H2208, m. 216-18', yellow, supposedly a dehydrated III, by
boiling with MeOH-HCI. I with ale. H2SO4 gave the Me ester. C27H2409,
yellow, m. 188-190', reconverted to I by hydrolysis and converted
to the Me ether, m. 22O-2', by CH2N2, then further to III by
hydrolysis. I gave the acetate. C3H28013, m. 222-4', by
acetylation and the Me ether Me ester (IV), C3OH3009, m. 221-2',
different from II, with MeZSO4. IV had no carbonyl group other than one
in the y-pytone ring, since IV did not form the oxime under mild
conditions. IV was hydrolyzed to a flavonecarboxylic acid Me ether (V),
C29H2809, m. 298'. converted to the Et ester, C3H3209, m.
208-210', by treating with alc. HCI. In an attempt to
decarboxylate by boiling with quinoline and Cu, IV was recovered unchanged
or decomposed, indicating that the carboxy group in IV was not attached to
the double bond. Heating V at 305' 7-8 min, gave the flavone
lactone (VI), C27H2208, m. 215-16', by demethylation and
dehydration, green with FeCl3. VI yielded the acetate, C29H2409, m.
185-7'. Hydrolysis of VI with 5% alc. KOH gave a flavonecarboxylic
acid (VII), C27H2208, m. 215-16', by demethylation and
dehydration, green with FeCl3. VI yielded the acetate, C29H2409, m.
185-7'. Hydrolysis of VI with 5% alc. KOH gave a flavonecarboxylic
acid (VII), C27H2208, m. 215-16', by demethylation and
ether gave a flavonecarboxylic acid Me ether (VIII), m. 297-8'.
VIII kept at 305' 5-7 min. gave the lactonic flavone t

IV). Demethyl derivative of Ia, m. above 320\*, gave demethyl derivative of I, which yielded IV with MeSO4. The structure of Ia was supposed to be a flavone nuclearly fused with a hydroflavonol.

114696-94-5 114791-94-5 115099-95-1-9

(Derived from data in the 6th Collective Formula Index (1957-1961))

114696-94-5 CAPLUS

4H-1-Benzopyran-6-acetic acid, a,5-dihydroxy-7-methoxy-a-p-methoxybenzyl-2-(p-methoxyphenyl)-4-oxo-, methyl ester (6CI) (CA INDEX NAME) ΙT

L4 ANSWER 140 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1961:17916 CAPLUS
DN 55:17916
OREF 55:3578i, 3579a-b
TI The structure of ginkgetin. IV. Alkali cleavage of ginkgetin
AU Kogure, Akira
CS Osaka City Univ.
SNippon Kagaku Zasshi (1959), 80, 1355-8
CODEN: NPKZAZ; ISSN: 0369-5387
DT Journal

CODEN: NPKZAZ; ISSN: 0369-5387

Journal

Unavailable

Ginkgetin (I) boiled 40 min. in 30% aqueous KOH solution gave

p-methoxyacetophenone (II), anisic acid (III), flavonecarboxylic acid

(IV), C25H2909, m. 308-10°, and cxoflavone (V), m. 269°

(decomposition). I boiled in 40% aqueous KOH solution many hrs. gave

ic acid, II,

III, and phloroglucinol. IV, C25H2009, brown with FeCl3, red with HCl-Mg,

was converted to the Me ether Me ester, C28H2609, m. 214-15°, brown

with FeCl3. V gave the oxime, m. 275-6°, and the semicarbazone, m.

228-30°. V gave the mono-Me ether, C27H2207, m. 220-2°,

green with FeCl3, converted to the acetate, C29H2409, m. 224-6.5°.

IV and V exhibited ultraviolet absorption essentially identical with that

of I.

of I.

114696-94-5 114791-94-5 115099-51-9

(Derived from data in the 6th Collective Formula Index (1957-1961))

114696-94-5 CAPLUS

4H-1-Benzopyran-6-acetic acid, a,5-dihydroxy-7-methoxy-a-p-methoxybenzyl-2-(p-methoxyphenyl)-4-oxo-, methyl ester (6CI) (CA INDEX NAME)

114791-94-5 CAPLUS
4H-1-Benzopyran-6-acetic acid, a,5,7-trihydroxy-a-p-hydroxybenzyl-2-(p-methoxyphenyl)-4-oxo-, ethyl ester (6CI) (CA INDEX NAME)

115099-51-9 CAPLUS 4H-1-Benzopyran-6-acetic acid, a,5-dihydroxy-7-methoxy-a-p-methoxybenzyl-2-(p-methoxyphenyl)-4-oxo-, ethyl ester (6CI) (CA INDEX NAME)

L

ANSWER 141 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) dihydroxyphenyl) butyric acid (XIII), 220-1", β-(2-methoxy-5-methylphenyl)-β-(2,4-dimethoxyphenyl) butyric acid (XIV) (8 g. from 15 g. of XIII), 116", 165", - (b10 240"); 10 g. IV, 10 g. resorcinol, 10 g. hydroxybutyrolactione of β-(2-methoxy-4-methylphenyl)-β-(2,4-dimethoxyphenyl) butyric acid (XV), 190" (methoxy deriv., m. 183"), β-(2-methoxy-4-methylphenyl)-β-(2,4-dimethoxyphenyl) butyric acid (XVI), 116-17", 132", - (b15 160"). Both, β,β-bis (ρ-methoxyphenyl) butyric acids, as well as β-(p-methoxyphenyl)-β-(o-methoxyphenyl) butyric acids, on distn. with lime at 3 mm. lost a mol. of AcOH and gave α,α-bis(substituted-phenyl)-β-(o-methoxyphenyl)-β-(o-methoxyphenyl)-g. (acids. The following were the results of distn. with lime of the various butyric acid derivs. preduct obtained, m.p. given): III, α,α-bis(4-methoxy-3-methylphenyl)-α'-(4-methoxy-3-methylphenyl)-α'-(4-methoxy-4-methylenyl)-α'-(4-methoxy-4-methylphenyl)-α'-(4-methoxy-4-methylenyl)-α'-(4-methoxy-4-methylenyl)-α'-(4-methoxy-4-methylenyl)-α'-(4-methoxy-4-methylenyl)-α'-(4-methoxy-4-methylenyl)-α'-(4-methoxy-4-methylenyl)-α'-(4-methoxy-4-methylenyl)-α'-(4-methoxy-4-methylenyl)-α'-(4-methoxy-4-m

L4 ANSWER 141 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1960:56237 CAPLUS
DN 54:56237
DN 54:56237
SHEP 54:10941d-1,10942a-d
TI Elimination of acetic acid during decarboxylation of organic acids. II.
Fornation of α,α-diarylethylenes from β,β'diarylbutyric acids
AU Gogte, G. R.: Xasaralkar, D. Y.
Inst. Sci., Bombay
Journal of the University of Bombay, Science: Physical Sciences,
Hathematics, Biological Sciences and Medicine (1958), 27(No. 3), 41-54
CODEN: JUBSAS: ISSN: 0368-4644
Journal
LA Unavailable
Ab cf. C. A. 54, 8717b. The preparation of variously substituted
β, β-diarylbutyric acids and their behavior on distillation with lime
was described. A mixture of 32 cc. AccHZCOZET (1) and 31 cc. o-cresol He
ether (II) cooled to 0-5', 200 cc. 70% HZSO4 added gradually with
shaking, the mixture left 8 hrs. at room temperature, poured on crushed ice
and
the semisolid lump hydrolyzed by refluxing 2 hrs. with 160 cc. aqueous 30%
NaOR and 100 cc. HeOH gave 16 g, β, β-bis(4-methoxy-3methylphenyl)butyric acid (III), m. 127'; antilde m. 143';
Et ester, m. 65'. Z-Methoxy-4-methyl-β-methylpinnyl)butyric
acid (IV), m. 139' (EtOH), obtained by an alkaline hydrolysis of
4,7-dimethylcoumarin, similarly condensed with II and anisole, resp., gave
β-[2-methoxy-4-methylphenyl)]butyric
acid (V), m. 120-1' (antilde m. 139'; Et ester m.
62'), and β-[2-methoxy-4-methylphenyl)-β-(4methoxyphenyl)butyric acid (VII), (McWers, C.A. 11, 2325) condensed with 24
cc. anisole gave 19 g. β-[2-methoxy-5-methylphenyl)-β-(4methoxyphenyl)butyric acid (VII), (McWers, C.A. 11, 2325) condensed with 24
cc. anisole gave 19 g. β-(2-methoxy-5-methylphenyl)-β-(4methoxyphenyl)butyric acid (VII), (McWers, C.A. 11, 2325) condensed with 24
cc. p-cresol gave 5 g. butyrolactone of β-(2-methoxy-5-methylphenyl)-β-(4methoxyphenyl) butyric acid (XII), m. 163';
Et ester hi? 70''. However, 10 g. VII condensed likewise with 6
cc. p-cresol gave 5 g. butyrolactone obtained, m.p., the corresponding
butyric acid (Writh (Allows), and the m. 117'; Et
ester m.

L4 ANSWER 142 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1960:11194 CAPLUS
DN 54:11194
OREF 54:2242c-i,2243a-d
T1 Thyroxine analogs. I. Synthesis of 3,5-dicodo-4-(2-alkylphenoxy)-OLphenylalanines
A Zenker, Nicolas: Jorgensen, Eugene C.
Univ. of California, San Francisco
OJ Journal of the American Chemical Society (1959), 81, 4643-7
CODEN: JACSAT: ISSN: 0002-7863
JOURNAL JORGAT: ISSN: 0002-7863
A series of compds. of the type named in the heading was prepared for
testing as analogs of thyroxine. 4,3,5-(p-MecGH4SO3)(OZN)ZCGHZCHZCH(NNAC)
COZET (I) (29.7 g.), m. 159-60.5' (aqueous MeZCO), 16 cc. dry CSH5N,
and 80 cc. dry CHCl3 refluxed 0.5 hr. the mixture treated with 0.09-0.42
boole appropriate o-alkylphenol, refluxed 2-6 hrs., cooled, washed, dried,
and evaporated, and the residue recrystd. or chromatographed on Al203
yielded

telded
the corresponding 4,3,5-ArO(OZN)2CGH2CH2CH(NHAC)CO2Et (II) (Ar, moles phenol and I used, reflux time in hrs., 1 yield, and m.p. given):
o-MeCGH4, 0.18, 0.06, 2.5, 58, 127-8\*; 2,4-Me2CGH3, 0.09, 0.09, 0.03, 2, 52, 120-2\*; 2,5-Me2CGH3, 0.18, 0.06, 3.5, 51, 112-13\*;
4,2,3-C1Me2CGH2, 0.11, 0.04, 7, 55, 139-40\*; 4,2,5-C1Me2CGH2, 0.11, 0.04, 7, 53, 168-9\*; o-iao-PrCGH4, 0.20, 0.03, 3.5, 46, 107-8\*; 2,5-iso-PrMeCGH3, 0.42, 0.06, 6, 43, 142-4\*;
2,4-Me(MeO)CGH3, 0.28, 0.10, 4, 63, 124-5\*; 2,5,4-Me2-(MeO)CGH2, 0.13, 0.05, 4, 51, 152-3\*; 2,4-iso-Pr(MeO)-CGH3, 0.15, 0.05, 8, 51, 105-6\*; 2,5,4-iso-PrMeCGH0O)CGH22, 0.14, 0.05, 8, 56, 160-2\*; The appropriate II (4.9 moles) refluxed 2 hrs. with 23 cc. glacial AcOH and 23 cc. concentrated HC1, diluted with 100 cc. H2O, adjusted to pH 5.0 ith 2N

ith 2N

NaOB, and filtered, and the residue repptd. from AcOH-HCl at pH 5.0, and recrystd. from aqueous CSHSN yielded the corresponding 4,3,5ArO(OZN)2CGH2CHCH(NH2)CO2H (Ar, N yield, and m.p. given): o-MeCGH4, 23, 192-3" (hygroscopic): 2,5-Me2CGH3, 13, 211-14",
o-iso-PrCGH4, 8, 187-90"; 2,5-iso-PrMeCGH2, 60, 196-9". The appropriate II (0,02 mole) in 300 cc. AcOH hydrogenated 45 min. at 35 lb. initial pressure over 2.0 g. 101 Pd-C, treated with 15 cc. concentrated 504,

filtered, added with stirring during 2 hrs. to 5.6 g. NaNO2 in 120 cc. concentrated H2SO4 and 40 cc. AcOH at -5°, stirred 2 hrs. at -5°, treated with stirring at 25° with 17 g. iodine and 12 g. NaI in 300 cc. H2O underlayered by 300 cc. CHCl3, the aqueous phase extracted after 2

with CHCl3, and the combined CHCl3 solns, worked up yielded the corresponding 3,5,4-12(ArO)CGH2CH2CH(NHAC)CO2Et (111) (Ar. % yield, and m.p. given): o-MeCGH3, 61, 111-12' (aqueous EtOH): 2,4-Me2CGH3, 55, 139-40' (aqueous EtOH): 2,5-Me2CGH3, 33, 147-8' (aqueous Me2CO): 4,2,3-CLMe2CGH2, 57, 175-6' (aqueous EtOH): 4,2,5-CLMe2CGH2, 61, 153-4' (aqueous EtOH): o-iso-PrCGH4, 57, 142-3' (aqueous Me2CO): 2,5-iso-PrMeCGH3, 65, 178-9' (aqueous EtOH): 2,4-Me(MeO)CGH3, 57, 150-1' (aqueous EtOH): 2,5-Me2(MeO)CGH2, 52, 163-40' (aqueous EtOH): 2,5-Me2(MeO)CGH2, 52, 163-40' (aqueous EtOH): 2,5-Me2(MeO)CGH2, 52, 163-40' (aqueous EtOH): The appropriate 111 (4.1 mmoles), 25 cc. glacial AcOH, and 25 cc. concentrated HCl refluxed

hrs., cooled, adjusted to pH 5.0 with 2N NaOH, and filtered, the residue dissolved in hot aqueous pyridine and repptd. with 2N HCl at pH 5, the report.

reppin.
repeated, and the crude product again repptd. from N NaOH in 50 or 75%

1

ANSWER 142 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) EtOH at pH 5.0 with 2N HCl in the presence of a few drops 2N NaOAc yielded the corresponding 3, 5.4-12 (ArO) CERIZCHZCH(NHZ) COZH (IV) (Ar, 1 yield, and m.p. with decompn. given): o-MecGH4. 87, 234-77; 2,4-Me2CGH3, 88, 190-2\*; 2,5-Me2CGH3, 56, 196-7\*; 4.2,3-CLMe2CGH2 (crystg. with 1 mole H2O), 71, 213-14\*; 4.2,5-CLMe2CGH2 (crystg. with 1 mole H2O), 71, 213-14\*; 4.2,5-CLMe2CGH2 (crystg. with 1 mole H2O), 71, 205-7\*; 0-iso-PrCGH4, 50, 202-5\*; 2,5-iso-PrMeCGH3, 78, 183-5\*. The appropriate III (9.5 mmoles), 40 cc. glacial AcOH, and 30 cc. 581 HI refluxed 8 hrs., concd. to near dryness at 50\*/5 mm, dissolved in a suspension of Na2S2O5 in hot EtOH, treated with addnl. Na2S2O5 until decolorized, adjusted with 2N NaOAc to pH 5.0, and centrifuged, and the ppt. repptd. from NaOH in 50t EtOH at pH 5.0 with 2N HCl gave the corresponding IV (Ar, 1 yield, and m.p. with decompn. given): 2,4-Me(H0)CGH3 (V), 67, 227-9\*; 2,5,4-Me2(H0)CGH2 (VII), 87, 199-201\*; 2,4-iso-Pr(H0)CGH3 (VIII), 87, 184-6\*; 2,5,4-iso-Pre(H0)CGH2 (VIII), 87, 190-1\*; V (2.0 g.) in 40 cc. 331 aq. EtNH2 treated with 5.1 cc. aq. soln. of 2.55 g. iedine and 4.0 g. XI during 2 hrs. at room temp., stirred 1 hr., adjusted to pH 5 with AcOH, and centrifuged, and the ppt. repptd. 3 times from N NaOH in 50t EtOH at pH 5.0 with 2N HCl contg. a few drops aq. NaOAc, washed, and centrifuged yielded 2.3 g. 5\*-iodo deriv. (1X) of V, light tan powder, m. 221-4\* (decompn.). VII (1.5 g.) in 25 cc. 331 aq. EtNH2 treated during 2 hrs. at room temp. with 5.3 cc. aq. soln. of 2.7 g. iodine and 4.1 g. KI, stirred 1 hr., and worked up in the usual manner gave only an incompletely iodinated material: a similar run during 9 hrs. resulted in less complete iodination than before. VI (0.52 g.) in 20 cc. 331 aq. EtNH2 treated during 1 hr., with 2.0 cc. aq. soln. of 1.0 g. iodin and 1.3 g. KI, stirred 1 hr., and worked up in the usual manner gave an incompletely iodinated product. VI (0.75 g.) in 5 cc. glacial AcOH stirred 1 h

Optived from data in the 6th Collective Formula Index (1957-1961)) 97116-28-4 CAPLUS Succinic acid, 2,3-di-o-tolyl-, diethyl ester (6CI, 7CI) (CA INDEX NAME)

L4 ANSWER 143 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN

ANSWER 143 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1960:11193 CAPLUS 54:11193 54:2241h-i,2242a-c Action of sodamide on α-bromoarylacetates Hoch, Joseph: Choisy, Jean M. Compt. rend. (1959), 248, 3314-16 Journal Unavailable Unavailable CASREACT 54:11193 Unavailable
CASREAT 54:11193
The appropriate Grignard reagent reacted with (COZEt)2 to give the following Et esters (% yield, b15, m.p. given): p-toluoylformate (I), 41, 155', 132', m-toluoylformate (II), 24, 150', 112'; o-toluoylformate (III), 26, 155', 154'; p-methoxybenzoylformate (IV), 38, 185', 152'; p-methoxybenzoylformate (IV), 38, 185', 128'; o-methoxybenzoylformate (IV), 38, 183', 117'; a-maphthoylformate (IV), 34, 203', 208'. I-VI were reduced by Al amalgam in moist Et20 to give, reap.: Et p-methylmandelate (VII), 824, b15 167', m. 77'; Et m-methylmandelate (VIII), 53%, b15 153'; Et c-methylmandelate (XI), 67%, b15 152'; Et p-methoxymandelate (X), 63%, m. 46'; Et o-methoxymandelate (XII), 70%, b10 170'; Et l-a-hydroxymaphthoylacetate (XII), 50%, m. 67'. Treatment of 3 moles each of VII-XII with 2 moles Pfr3 in warm Gelid solution converted them to the following: Et p-tolyl-a-bromoacetate (XIII), 51%, b30 177'; Et m-tolyl-a-bromoacetate (XIV), 33%, b15 155-6'; Et o-tolyl-a-bromoacetate (XVI), 45%, b15 153-6'; Et p-methoxyphenyl-a-bromoacetate (XVII), 56%, b1 130-40'; and Et l-naphthyl-a-bromoacetate (XVIII), 40%, b2 185'. The bromoacetates were treated with NaNB2 (Vavon and Antonini, C.A. 45, 5821) and the products separated and identified. XIII 60% material, b15 240-50', which was di-Et di-p-tolylmaleate, m. Antonini, C.A. 45, 58/1) and the products separated and identified. Al 60% material, bl5 240-50°, which was di-Et di-p-tolylmaleate, m. 84°, and di-Et di-p-tolylfumarate, m. 117°. From the non-orystallizable residue, after saponification, there was obtained di-p-tolylmaleic anhydride and di-p-tolylmaleic acid. XIV gave di-Et di-m-tolylmaleic anhydride, m. 92-3°, and di-m-tolylfumaric acid, m. 265°. XV gave a fraction, bl5 215-40°, which yielded a small amount di-Et di-o-tolylsuccinate, m. 149°. XVII resected difficultly and gave noncryst. products which on saponification gave a trace of di-o-methoxyphenylmaleic anhydride, m. 162°. XVIII gave only resinous products.
97116-28-47, Succinic acid, 2,3-di-o-tolyl-, diethyl ester (Preparation of) 97116-28-4 CAPLUS Succinic acid, 2,3-di-o-tolyl-, diethyl ester (6CI, 7CI) (CA INDEX NAM

Succinic acid, 2,3-di-o-tolyl-, diethyl ester (6CI, 7CI) (CA INDEX NAME)

ANSWER 144 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1959:114554 CAPLUS 53:114554

53:20554d-e
Pharmacology of organic acid esters and amides
Oyaizu, Susumu
Univ. Kyoto
Yakugaku Kenkyu (1958), 30, 108-19
CODEN: YKKKA8; ISSN: 0372-7734
Journal
Unavailable
Unavailable Unavailable
Pharmacol. action of over 20 derivs. of dimethylaminoethyl diphenylacetate and diphenylglycolate was examined for possible relation between chemical structure and pharmacol. activity. No definite relation was found except in atropine activity; the activity was generally weakened by substitution of one of the Ph groups with benzyl, substitution of the base with a heterocylic system, substitution of the phenyl with Cl or MeO at the para position, and derivation of the ester to its amide. Atropine activity increased by quaternization of the base, and substitution of dimethyl in the base with diethyl.
109095-40-1, Lactic acid, 2,3-bis(p-chlorophenyl)-,
2-dimethylaminoethyl ester (pharmacology of)
109095-40-1 CAPLUS
Lactic acid, 2,3-bis(p-chlorophenyl)-, 2-dimethylaminoethyl ester (6CI) (CA INDEX NAME)

L4 ANSYER 145 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN AN 1956:77742 CAPLUS ON 50:77742 CAPLUS OREF 50:16664f-i,14665a-c TI Nitrogen containing designs. SU: //W4
SU: own product, b1-2 76-102°, and 2.8 g. viscous oil, b1-2 165-78°, which gave 0.5 g. I. To 2.4 g. Na in 65 ml. EtOH was added 19.3 g. molten Ph2CHCM and 15 ml. EtOH, the solution was chilled and treated over 20 min. with 24.3 g. EtO2CCHEPTh and 20 ml. EtOH; after 0.5 hr. the mixture was stirred 1 hr. with cooling and kept overnight; the precipitate was filtered and washed with H2O yielding 66.8% Ph2C(CN)CHPhCO2Et, m. 164-5° (crude), m. 165-6° (from EDOH). Hydrolysis of 75 g. (PhCHCN)2 according to Wavzonek (C.A. 34, 3730.3) followed by separation of the resulting acid and conversion to the Ba salt gave a precipitate of racemic salt, while the filtrate containing the Ba salt of the meso form was heated 70° and acidified with HCl yielding 73.1% meso-(PhCHCO2H)2, m. . 227-9°. Boiling the Ba salt of the racemate with dilute H2SO4 and separation of BaSO4 gave on cooling 19.7% racemic (PhCHCO2H)2 monohydrate, Separation or sacw gave on cooling 19.7% facemate (FRCHCUZH)2 monohydrate, 183-5°. Refluxing I with 1:1 H2SO4 and ACOH 7 hrs.. gave some EtoAc: the residue was refluxed 6 hrs. with more ACOH and diluted yielding 92.3% meso-(FNCHCUZH)2, m. 227-9°, which (37.8 g.) with 59.5 g. PCL5 and 40 Pnt-PCL3 gave on heating to 100° 75.1% meso-(FNCHCUCH)2, m. 186-8°, which refluxed with EtOH gave the di-Et ester, m. 140-17; Me2NCHZHOH similarly gave the bis(dimethylaminoethyl) ester (II), m. 93-5° (di-HCl salt, m. 239-40°); similarly was prepared bis(diethylaminoethyl) ester (III), m. 58-60° (di-HCl salt, m. 205-6°). Il treated with MeI in MeZCO gave the dimethiodide, m. 225-6°. To 50 ml. HNO3 (d. 1.52) was added with cooling 10 g. meso-(FNCHCUCH)2 at about 0° in 1 hr. and after stirring 0.5 hr. the mixture was quenched with ice, the separated product dried and boiled 1 with 200 ml. AcOH and filtered hot yielding 8.5 g. solid, m. 227-8°, which was taken up in aqueous MH40H, decolorized and treated with hot AcOH yielding 56.4% meso-(p-02NC6H4CHCO2H), g. m. 238-40°; this with EtOH-H2SO4 gave after 27 hrs. refluxing 38.8% di-Et ester, m. 159-61°; the same was obtained in 62.7% yield on nitration of the unsubstituted ester above with HNO3 (d. 1.51) at about 0°.

Journal of Pharmacology and Experimental Therapeutics (1954), 112, 176-84 CODEN: JPETAB: ISSN: 0022-3565 Journal Unavailable A series of 35 diarylalkanes (not named) were tested for depressor activity in renal hypertensive rats and in rats with metacorticoid hypertension produced by subcutaneous implantation of 20 mg. of decoxycorticosterone acetate. A significant and approx. equal activity was shown by 2,3-bis(p-hydroxyphenyl)-valeronitrile (I) and the corresponding propionitrile (II). I also displayed estrogenic activity, growth inhibition, and stimulation of adrenal hypertrophy in normotensive rats, and in large doses induced severe hemorrhapic responses in dogs. The corresponding effects of II, if any, were slight. Replacement of the nitrile group of I by CODH, COME, CODE, COME, or CH2NH2-HBr greatly reduced the depressor activity.

857479-98-2, Valeric acid, 2,3-bis(p-hydroxyphenyl)-, ethyl ester (depressor activity of) 857479-98-2 CAPLUS Valeric acid, 2,3-bis(p-hydroxyphenyl)-, ethyl ester (SCI) (CA INDEX NAME)

ANSWER 145 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) Reduction of the ester with SnC12 2H20 in EtOH in the presence of Ca gave in 5 hrs. 70.2% meso-(p-H2NC6H4CHCO2E1)2, m. 183-5" (crude); m. 186-7" (from CGH6); without added CaCO3 the reaction tends to give a low melting product. This refluxed with Mel in EtOH in the presence of H20 and CaCO3 5 hrs. gave the dimethiodide, m. 212-14" (from H20). The 3 methiodides described above showed curare-like properties.
860426-35-3P, Succinic acid, 2,3-bis(p-aminophenyl)-, diethyl ester

ester RL: PREP (Preparation)

(preparation of)
860426-35-3 CAPLUS
Succinic acid, 2,3-bis(p-aminophenyl)-, diethyl ester (5CI) (CA INDEX NAME)

=> file reg COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION 491.44 FULL ESTIMATED COST 664.17 DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION CA SUBSCRIBER PRICE -71.76 -71.76

FILE 'REGISTRY' ENTERED AT 10:03:52 ON 27 DEC 2007 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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STRUCTURE FILE UPDATES: 26 DEC 2007 HIGHEST RN 959588-76-2 DICTIONARY FILE UPDATES: 26 DEC 2007 HIGHEST RN 959588-76-2

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and

1:Atom 2:CLASS 3:CLASS 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:CLASS 16:CLASS 17:CLASS 19:CLASS 20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 29:CLASS 30:Atom 31:CLASS 32:Atom

L5 STRUCTURE UPLOADED

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100.0% PROCESSED 148 ITERATIONS

19 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*
BATCH \*\*COMPLETE\*\*

2231 TO

PROJECTED ITERATIONS: PROJECTED ANSWERS: 119 TO

L6 19 SEA SSS SAM L5

=> d scan

L6 19 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN Benzenepropanamide, 4-(aminoiminomethyl)-N-[(15)-1-cyclohexyl-2-[[[1-(1-ininotethyl)-4-piperidinyl]methyl]amino)-2-oxoethyl]-α-[3-(trifluoromethyl)phenyl]-, (α5)C1 COM

Absolute stereochemistry.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):END

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Executing the logoff script...

=> LOG H

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.45	664.62
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
CA SUBSCRIBER PRICE	ENTRY	SESSION -71 76

SESSION WILL BE HELD FOR 120 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 10:04:35 ON 27 DEC 2007

=> d his

(FILE 'HOME' ENTERED AT 08:08:15 ON 27 DEC 2007)

FILE 'REGISTRY' ENTERED AT 08:08:27 ON 27 DEC 2007

L1 STRUCTURE UPLOADED

L2 1 S L1

L3 1 S L1 CSS

L4 1 S L1 CSS FUL

FILE 'REGISTRY' ENTERED AT 08:17:29 ON 27 DEC 2007

L5 1 S L1

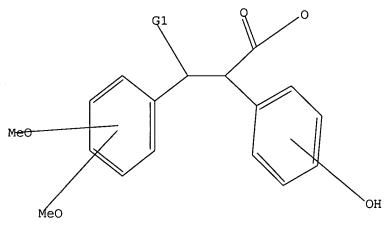
L6 5 S L1 FUL

FILE 'CAPLUS' ENTERED AT 08:17:45 ON 27 DEC 2007

=> d 11

L1 HAS NO ANSWERS

L1 STR



G1 H, Ak, CH

Structure attributes must be viewed using STN Express query preparation.

=> s 16

L7 12 L6

=> d bib abs hitstr 1-12

L7 ANSWER 1 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2003:757334 CAPLUS

DN 139:276885

TI Preparation of novel heterocyclic analogs of diphenylethylene compounds as antidiabetics

IN Neogi, Partha; Dey, Debendranath; Medicherla, Satyanarayana; Nag, Bishwajit; Lee, Arthur

PA USA

SO U.S. Pat. Appl. Publ., 66 pp., Cont.-in-part of U.S. Ser. No. 843,167. CODEN: USXXCO

DT Patent

LA English

FAN. CNT 12

PATENT NO. KIND DATE APPLICATION NO. DATE

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                                20031008
OS
    MARPAT 139:276885
GI
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### \* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB The title compds. [I; Z = II-IV; n, m, q and r = 0-4 ( $n+m \le 4$  and  $q+r \le 4$ ); p, s = 0-5 (p+s  $\le$  5); R, R2 = H, alkyl, alkenyl, etc.; R1 = H, alkyl, alkenyl, etc.; A, A1, A2 = H, acylamino, acyloxy, alkanoyl, etc.; B, B1, B2 = H, acylamino, acyloxy, alkanoyl, etc.; or A and B together, or A1 and B1 together, or A2 and B2 together, may be joined to form a methylenedioxy or ethylenedioxy; X, X1 = (un)substituted NH, O, S] which are effective in lowering blood glucose level, serum insulin, triglyceride and free fatty acid levels in animal models of Type II diabetes, were prepared E.g., a multi-step synthesis of V, starting from 3,5-dimethoxybenzaldehyde and 4-hydroxyphenylacetic acid, was given. The compound V showed strong glucose lowering activity even though it is a weak PPAR- $\gamma$  agonist (data given). The compds. I are disclosed as useful for a variety of treatments including the treatment of inflammation, inflammatory and immunol. diseases, insulin resistance, hyperlipidemia, coronary artery disease, cancer and multiple sclerosis. Pharmaceutical composition comprising the compound I was claimed.

IT 380881-43-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of diphenylethylene compds. containing thiazolidinedione or oxazolidinedione moieties for treating diabetes, inflammatory or immunol. disease in combination with other agents)

RN 380881-43-6 CAPLUS

CN Benzenepropanoic acid,  $\alpha$ -(4-hydroxyphenyl)-3,5-dimethoxy-, methyl ester (CA INDEX NAME)

L7 ANSWER 2 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2003:645701 CAPLUS

DN 140:87046

TI Synthesis and structure-Activity relationship studies of cinnamic acid-based novel thiazolidinedione antihyperglycemic agents

AU Neogi, Partha; Lakner, Fredrick J.; Medicherla, Satyanarayana; Cheng, Jin; Dey, Debendranath; Gowri, Maya; Nag, Bishwajit; Sharma, Somesh D.; Pickford, Lesley B.; Gross, Coleman

CS Department of Chemistry, Calyx Therapeutics Inc., Hayward, CA, 94545, USA

SO Bioorganic & Medicinal Chemistry (2003), 11(18), 4059-4067 CODEN: BMECEP; ISSN: 0968-0896

PB Elsevier Science Ltd.

DT Journal

LA English

OS CASREACT 140:87046

GI

MeO CO CH OMe OMe 
$$p$$
-C6H4  $CH_2$ 

Ι

AB A number of 2,4-thiazolidinedione derivs. of -Ph substituted cinnamic acid were synthesized and studied for their PPAR agonist activity. The E-isomer of cinnamic acid, I, showed moderate PPAR transactivation. The corresponding Z-isomer and double bond reduced derivative were found to be much less potent. Although the E-isomer showed a moderate PPARy transactivation, it demonstrated a strong glucose-lowering effect in a genetic rodent model of diabetes. Results of pharmacokinetic, metabolism and permeability studies are consistent with I being an active prodrug with the hydrolyzed carboxylate as an active metabolite that has similar

glucose lowering and PPARy agonist properties.

380881-43-6P IT

> RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(cinnamic acid-based thiazolidinedione antihyperglycemic agents)

RN 380881-43-6 CAPLUS

CN Benzenepropanoic acid,  $\alpha$ -(4-hydroxyphenyl)-3,5-dimethoxy-, methyl ester (CA INDEX NAME)

#### RE.CNT 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 3 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2002:185699 CAPLUS

136:247571 DN

Preparation of novel heterocyclic analogs of diphenylethylene compounds as ΤI inhibitors of cytokines or cyclooxygenase

Nag, Bishwajit; Dey, Debendranath; Medicherla, Satyanarayana; Neogi, IN Partha

PΑ Theracos, Inc., USA

SO U.S. Pat. Appl. Publ., 34 pp., Cont.-in-part of U.S. Ser. No. 785,554. CODEN: USXXCO

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	US 7202366	B2	20070410		
PRAI	US 1998-74925	A2	19980508		
	US 1999-287237	A2	19990406		
	US 2000-591105	A2	20000609		
	US 2001-785554	A2	20010220		
	US 2001-843167	A	20010427		
	WO 2001-US17950	W	20010605		
OS	MARPAT 136:247571				
GI					

$$Q = \begin{bmatrix} A_p & A_q & A_p & R \\ B_{p1} & B_{q1} & B_{p1} & B_{p1} \end{bmatrix}$$

AB Novel diphenylethylene compds. and derivs. thereof containing thiazolidinedione or oxazolidinedione moieties are provided which are effective in lowering blood glucose level, serum insulin, triglyceride and free fatty acid levels in animal models of Type II diabetes. The above compds. and their derivs. are resented by formula [I; Z = Q, Q1, H, A", B"; wherein n, m, q, q1 = integers from zero to 4 provided that  $n+m\leq 4$  and  $q+q1\leq 4$ ; p, p1 = integers from zero to 5 provided that p+p1≤5; a, b and c are double bonds which may be present or absent; when present; the double bonds may be in the E or Z configuration and, when absent, the resulting stereocenters may have the R- or Sconfiguration; R, R', R" = H, C1-20 linear or branched alkyl, C2-20 linear or branched alkenyl, CO2Z' (wherein Z' = H, Na, K, or other pharmaceutically acceptable counterion such as Ca, Mg, ammonium, tromethamine, and the like), CO2R''', NH2, NHR''', N(R''')2, OH, OR''', halo, substituted C1-20 linear or branched alkyl or substituted C2-20 linear or branched alkenyl (wherein R''' is C1-20 linear or branched alkyl or linear or branched alkenyl); A, A', A'' = H, C1-20 acylamino, C1-20 acyloxy, C1-20 alkanoyl, C1-20 alkoxycarbonyl, C1-20 alkoxy, C1-20 alkylamino, C1-20 alkylcarboxylamino, CO2H, cyano, halo, HO; B, B', B'' = H, C1-20 acylamino, C1-20 acyloxy, C1-20 alkanoyl, C1-20 alkenoyl, C1-20 alkoxycarbonyl, C1-20 alkoxy, C1-20 alkylamino, C1-20 alkylcarboxylamino, aroyl, aralkanoyl, CO2H, cyano, halo, HO; or A and B together, or A' and B' together, or A'' and B'' together, may be joined to form a methylenedioxy or ethylenedioxy group; and X, X' are independently -NH, -NR''', O or S]. In contrast to previously reported thiazolidinedione compds., known to lower leptin levels, the present compds. increase leptin levels and have no known liver toxicity. They inhibit the activity of TNF-alpha, interleukin IL-1 or IL-6 or cyclooxygenase-2 (COX-2). The

compds. are disclosed as useful for a variety of treatments including the treatment of inflammation, inflammatory and immunol. diseases, insulin resistance, hyperlipidemia, coronary artery disease, cancer and multiple sclerosis. Thus, To a mixture of 3,5-dimethoxybenzaldehyde (500 g) and p-hydroxyphenylacetic acid (457 q) was added acetic anhydride (1 L) and triethylamine (420 mL) and the nonhomogeneous mixture on heating became homogeneous at 70° and stirred at 130-140° for 6 h to give 47% 3-(3,5-dimethoxyphenyl)-2-(4-hydroxyphenyl)acrylic acid (II) (428 g). II (427.5 g) was suspended in 3 L methanol, treated with 100 mL concentrated H2SO4, and heated at reflux for 20 h under Ar to give 97% 3-(3,5-dimethoxyphenyl)-2-(4-hydroxyphenyl)acrylic acid Me ester (III). III (433 q) was dissolved in 1.6 L DMF, treated with 60.4 q NaH (50% in oil) and the with 185 mL p-fluorobenzaldehyde, and heated at 180° for 18 h to give 77% 3-(3,5-dimethoxyphenyl)-2-[4-(4formylphenoxy)phenyl]acrylic acid Me ester which (352 g), 2,4-thiazolidinedione 98.6, benzoic acid 134, and piperidine 107.4 g were heated in 2.5 L toluene at reflux with continuous removal of H2O through Dean-Stark apparatus to give 86% 3-(3,5-dimethoxyphenyl)-2-[4-[4-(2,4dioxothiazolidin-5-ylidenemethyl)phenoxy]phenyl]acrylic acid Me ester (IV). IV (30 q) was hydrogenated over 15 q 10% Pd-C in 900 mL dioxane in a Parr apparatus at 60 Psi for 24 h, followed by adding 15 g 10% Pd-C and continuing the hydrogenation for another 24 h to give 86% 3-(3,5-dimethoxyphenyl)-2-[4-[4-(2,4-dioxothiazolidin-5ylmethyl)phenoxy]phenyl]acrylic acid Me ester (V). When V was orally administered to ob/ob mice with a single oral dose (50 mg/kg body weight), there was a 62 % drop in blood glucose level and, similar to db/db mice, there was no significant increase in body weight between the control and the treatment groups. This was in contrast to treatment of diabetic animals by thiazolidinedione type compds. which are known to be associated with increase in body weight

IT 380881-43-6P, 3-(3,5-Dimethoxyphenyl)-2-(4-hydroxyphenyl)propionic acid methyl ester

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of novel heterocyclic analogs of phenylethylene compds. as inhibitors of cytokines or cyclooxygenase for therapeutic agents)

RN 380881-43-6 CAPLUS

CN Benzenepropanoic acid,  $\alpha$ -(4-hydroxyphenyl)-3,5-dimethoxy-, methyl ester (CA INDEX NAME)

RE.CNT 84 THERE ARE 84 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 4 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2002:11108 CAPLUS

DN 136:69654

TI Preparation of diphenylethylene compounds as antidiabetic agents

IN Nag, Bishwagit; Dey, Debendranath; Medicherla, Satyanarayana; Neogi, Partha

PA USA

SO U.S. Pat. Appl. Publ., 38 pp., Cont.-in-part of U.S. Ser. No. 642,618.

CODEN: USXXCO

DT Patent LA English

FAN.	CNT 12					
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	US 1999-436047	A3	19991108			
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	US 2001-334818P	P	20011129			
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	WO 2002-US38150	A2	20021127			
OS	MARPAT 136:69654					
GI						

$$R^{2}$$
 $R^{3}$ 
 $R^{4}$ 
 $R^{6}$ 
 $R^{5}$ 

AB Title compds. I [wherein A = CO2R, CONR'R", CN, or COR7; X = H, OH, or (un) substituted alkyl or alkenyl; R = H, (ar) alkyl, or aryl; R1, R2, R3, R4, R5, R6, and R7 = independently H, (un) substituted alkyl or alkenyl; CO2R, NR'R", or CONCR'R"; R' and R" = independently H, alkyl, aryl, OH, alkoxy, acylamino, acyloxy, alkanoyl, alkoxylcarbonyl, halo, NO2, SO2R'''; CZ3; Z = independently H, halo, (halo)alkyl, or SR'''; R''' = H or alkyl; or R2 and R3 together or R5 and R6 together may be joined to form (m)ethylenedioxy; with provisos; and E and Z isomers thereof] were prepared and shown to decrease circulating concns. of glucose when administered orally. For instance, 3,5-dimethoxybenzaldehyde was coupled with p-hydroxyphenyl acetic acid using TEA in acetic anhydride to give (E)-3-(3,5-dimethoxyphenyl)-2-(4-hydroxyphenyl)acrylic acid (II), which exhibited glucose-lowering effects for more than 15 days at a dose of 20 mg/kg p.o. Examples also include twenty-six bioassays, such as studies on the effects of II on insulin resistant rats, lipid and leptin concns., PPAR binding, overexpression of the human insulin-like growth factor 1 receptor and human insulin receptor, toxicity, and kinetics of drug absorption. I are orally effective antidiabetic agents that normalize glucose and lipid metabolism

IT 353228-00-9P

RN

CN

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation and testing of diphenylethylene antidiabetic agents that normalize glucose and lipid metabolism in relation to insulin resistance) 353228-00-9 CAPLUS

Benzenepropanoic acid,  $\alpha$ -(4-hydroxyphenyl)-3,4-dimethoxy- (CA INDEX

NAME)

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WO 2001-US17950

MARPAT 136:37596

OS

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20010605

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L7
     ANSWER 5 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN
AN
     2001:923567 CAPLUS
DN
     136:37596
ΤI
     Preparation and activity of diphenylethylene thiazolidinedione or
     oxazolidinedione compounds as antidiabetics or antiinflammatories
IN
     Neogi, Partha; Nag, Bishwajit; Medicherla, Satyanarayana; Dey,
     Debendranath
PA
     Calyx Therapeutics, Inc., USA
SO
     PCT Int. Appl., 76 pp.
     CODEN: PIXXD2
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     Patent
     English
LA
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     PATENT NO.
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                                             APPLICATION NO.
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                                             NZ 2001-522660
                                                                     20010605
     IN 2002CN01998
                          Α
                                 20050225
                                             IN 2002-CN1998
                                                                     20021204
     MX 2002PA12038
                          Α
                                 20031015
                                             MX 2002-PA12038
                                                                     20021205
PRAI US 2000-591105
                          A2
                                 20000609
     US 2001-785554
                          A2
                                 20010220
     US 2001-843167
                          A2
                                 20010427
     US 1998-74925
                          A2
                                 19980508
     US 1999-287237
                          A2
                                 19990406
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AB Novel diphenylethylene compds. and derivs. thereof containing thiazolidinedione or oxazolidinedione moieties are provided which are effective in lowering blood glucose level, serum insulin, triglyceride and free fatty acid levels in animal models of Type II diabetes. In contrast to previously reported thiazolidinedione compds., known to lower leptin levels, the present compds. increase leptin levels and have no known liver toxicity. Thus, (I) was prepared in five steps by condensation of 3,5-dimethoxybenzaldehyde with 4-hydroxyphenylacetic acid followed by esterification and etherification with 4-fluorobenzaldehyde and condensation with 2,4-thiazolidinedione and hydrogenation of the ylidene double bond. Oral administration of I to obese mice caused a 62% drop in blood glucose level. The compds. are disclosed as useful for a variety of treatments including the treatment of inflammation, inflammatory and immunol. diseases, insulin resistance, hyperlipidemia, coronary artery disease, cancer and multiple sclerosis.

IT 380881-43-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and activity of diphenylethylene thiazolidinedione or oxazolidinedione compds. as antidiabetics or antiinflammatories)

RN 380881-43-6 CAPLUS

CN Benzenepropanoic acid,  $\alpha$ -(4-hydroxyphenyl)-3,5-dimethoxy-, methyl ester (CA INDEX NAME)

L7 ANSWER 6 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2001:581654 CAPLUS

DN 135:147444

TI Novel diphenylethylene compounds

IN Nag, Bishwajit; Dey, Debendranath; Medicherla, Satyanarayana

PA Calyx Therapeutics, Inc., USA

SO PCT Int. Appl., 55 pp.

CODEN: PIXXD2

DT Patent

LA English FAN.CNT 12

	PATENT NO.				KIN	D	DATE			APPLICATION NO.					DATE			
ΡI	WO	WO 2001056382				A1		20010809		WO 2001-US3797						20010205		
		W:	ΑE,	AG,	AL,	AM,	AT,	AU,	ΑZ,	BA,	BB,	BG,	BR,	BY,	BZ,	CA,	CH,	CN,
			CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	ΕE,	ES,	FI,	GB,	GD,	GE,	GH,	GM,	HR,
			HU,	ID,	IL,	IN,	IS,	JP,	KΕ,	KG,	KP,	KR,	KZ,	LC,	LK,	LR,	LS,	LT,
			LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NO,	NZ,	PL,	PT,	RO,	RU,
			SD,	SE,	SG,	SI,	SK,	SL,	TJ,	TM,	TR,	TT,	TZ,	UA,	UG,	US,	UΖ,	VN,
			YU,	ZA,	ZW													
		RW:						MZ,										
			DE,	DK,	ES,	FI,	FR,	GB,	GR,	ΙE,	ΙT,	LU,	MC,	NL,	PT,	SE,	TR,	BF,
								GA,										
	CA 2397076					US 2000-642618												
							CA 2001-2397076											
	EΡ						EP 2001-905454 GB, GR, IT, LI, LU, NL											
		R:											LI,	LU,	NL,	SE,	MC,	PT,
					-	-		RO,	-	•								
	JP 2003521500 NZ 520829			Т		20030715 JP 2001-556090 20041224 NZ 2001-520829												
	NZ	5208	29			Α												
		7849						2006									0010	
		2002						2004										
		2002						2007			IN 2	002-	CN13	21		2	0020	822
PRAI		2000						2000										
		2000						2000										
		1998						1998										
0.5		2001		197		W		2001	0205									

OS MARPAT 135:147444

AB Novel diphenylethylene compds. that are administered orally to decrease circulating concns. of glucose are provided. The effect on insulin resistant rats is also shown. The effects on lipid and leptin concns. are also shown. The compds. are orally effective anti-diabetic agents that may normalize glucose and lipid metabolism in subjects with diabetes.

IT 353228-00-9P

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(novel diphenylethylene compds. that are anti-diabetic agents that normalize glucose and lipid metabolism in relation to insulin resistance) 353228-00-9 CAPLUS

CN Benzenepropanoic acid,  $\alpha$ -(4-hydroxyphenyl)-3,4-dimethoxy- (CA INDEX NAME)

$$\begin{array}{c|c} \text{OMe} & \text{OMe} \\ \hline \text{CO}_2\text{H} & \text{OMe} \\ \hline \text{CH-CH}_2 & \text{OMe} \\ \end{array}$$

RE.CNT 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 7 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1999:771171 CAPLUS

DN 132:122418

RN

TI Synthesis and biological evaluation of dihydrobenzofuran lignans and related compounds as potential antitumor agents that inhibit tubulin polymerization

AU Pieters, Luc; Van Dyck, Stefaan; Gao, Mei; Bai, Ruoli; Hamel, Ernest;

Vlietinck, Arnold; Lemiere, Guy

CS Department of Pharmaceutical Sciences, University of Antwerp, Belgium, B-2610, Belg.

Ι

SO Journal of Medicinal Chemistry (1999), 42(26), 5475-5481 CODEN: JMCMAR; ISSN: 0022-2623

PB American Chemical Society

DT Journal

LA English

GΙ

AB A series of 19 related dihydrobenzofuran lignans and benzofurans was obtained by a biomimetic reaction sequence involving oxidative dimerization of p-coumaric, caffeic, or ferulic acid Me esters, followed by derivatization reactions. All compds. were evaluated for potential anticancer activity in an in vitro human disease-oriented tumor cell line screening panel that consisted of 60 human tumor cell lines arranged in nine subpanels, representing diverse histologies. Leukemia and breast cancer cell lines were relatively more sensitive to these agents than were the other cell lines. Me (E)-3-[2-(3,4-dihydroxyphenyl)-7-hydroxy-3methoxycarbonyl-2,3-dihydro-1-benzofuran-5-yl]prop-2-enoate (I), the dimerization product of caffeic acid Me ester, containing a 3',4'-dihydroxyphenyl moiety and a hydroxyl group in position 7 of the dihydrobenzofuran ring, showed promising activity. The average GI50 value (the molar drug concentration required for 50% growth inhibition) of I was 0.3  $\mu M$ . Against three breast cancer cell lines, I had a GI50 value of <10 nM. Methylation, reduction of the double bond of the C3-side chain, reduction

of

the methoxycarbonyl functionalities to primary alcs., or oxidation of the dihydrobenzofuran ring to a benzofuran system resulted in a decrease or loss of cytotoxic activity. Compound I inhibited mitosis at micromolar concns. in cell culture through a relatively weak interaction at the colchicine binding site of tubulin. In vitro it inhibited tubulin polymerization

by 50% at a concentration of 13  $\pm$  1  $\mu M.$  The 2R,3R-enantiomer of I was twice as active as the racemic mixture, while the 2S,3S-enantiomer had minimal activity as an inhibitor of tubulin polymerization. These dihydrobenzofuran lignans (2-phenyl-dihydrobenzofuran derivs.) constitute a new group of antimitotic and potential antitumor agents that inhibit tubulin polymerization

IT 256330-13-9P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(synthesis and biol. evaluation of dihydrobenzofuran lignans and related compds. as potential antitumor agents that inhibit tubulin polymerization)

RN 256330-13-9 CAPLUS

CN Benzenepropanoic acid,  $\alpha$ -[2-hydroxy-3-methoxy-5-(3-methoxy-3-oxopropyl)phenyl]-3,4-dimethoxy-, methyl ester (CA INDEX NAME)

RE.CNT 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 8 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1966:429366 CAPLUS

DN 65:29366

OREF 65:5434e-f

TI Flavanoids. II. Stereochemistry of isoaurones

AU Marathe, K. G.; Byrne, M. J.; Vidwans, R. N.

CS Univ. Poona, India

SO Tetrahedron (1966), 22(6), 1789-95

CODEN: TETRAB; ISSN: 0040-4020

DT Journal

LA English

AB cf. CA 54, 3402a. Isoaurones (anhydrolactones of 2-hydroxy- $\alpha$ -benzylmandelic acids), trimethylanhydrohazeyl lactone and its 5-methyl-4'-methoxy analog are shown to be trans-stilbene derivs. and are isomerized to the cis compds. by pyridine. The stereochemistry has been established by a stereoselective synthesis of the derived cis-stilbene- $\alpha$ -carboxylic acid and confirmed by uv and N.M.R. studies. A mechanism for isomerization has been suggested.

IT 6600-62-0P, Lactic acid, 3-(3,4-dimethoxyphenyl)-2-(2-hydroxy-4-methoxyphenyl)-

RL: PREP (Preparation)

(preparation of)

RN 6600-62-0 CAPLUS

CN Lactic acid, 3-(3,4-dimethoxyphenyl)-2-(2-hydroxy-4-methoxyphenyl)- (7CI, 8CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{OH} & \text{CO}_2\text{H} \\ \hline \text{C} & \text{CH}_2 \\ \hline \text{OH} & \text{OMe} \end{array}$$

L7 ANSWER 9 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1966:93097 CAPLUS

DN 64:93097

OREF 64:17468f-h,17469a-b

TI Reaction of 2,6-and 2,4-xylenols with oxo acids

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IIA
    Merchant, J. R.; Mehta, J. B.
CS
     Inst. Sci., Bombay
     Indian Journal of Chemistry (1966), 4(2), 76-8
SO
     CODEN: IJOCAP; ISSN: 0019-5103
DT
     Journal
     English
LΑ
GΙ
     For diagram(s), see printed CA Issue.
AB
     cf. Parris, et al., CA 57, 723i; Smith and Bealor, CA 57, 12377q. Concentrated
    H2SO4 (5 ml.) was added dropwise with stirring to a mixture of 4.8 g.
     2,6-xylenol (I) and 1.76 g. pyruvic acid kept at 0-5°. After 30
     min., the mixture was poured into ice-cold H2O to yield 3 q.
     2,2-bis(3,5-dimethyl-4-hydroxyphenyl)propionic acid (II), m.
     201-2°. II was also obtained when dry HCl was passed through a
     mixture of the same amounts of the reactants in 10 ml. HOAc at 0-5°
     for 4 hrs. Similarly, condensation of 2.4 g. I with 1.64 g. phenylpyruvic
     add, 2.2 g. 3,4-dimethoxyphenylpyruvic acid, 1 g. dimethylpyruvic acid, 1
     g. \alpha-oxo-n-valeric acid, and 1.5 g. \alpha-oxoglutaric acid, resp.,
     in HOAc at 0-5° in the presence of HCl yielded 2 q.
     2,2-bis(3,5-dimethyl-4-hydroxyphenyl)phenylpropionic acid, m.
     239-40° (C6H6); 1 q. 2,2-bis(3,5-dimethyl-4-hydroxyphenyl)-
     3,4-dimethoxyphenylpropionic acid, m. 190-1° (dilute EtOH); 450 mg.
     2,2-bis(3,5-dimethyl-4-hydroxyphenyl)dimethylpropionic acid, m.
     250-1° (C6H66); 2,2-bis(3,5-dimethyl-4-hydroxy-
    phenyl)propylpropionic acid, m. 235-6° (C6H6); and 1 g. 2,2-
    bis(3,5-dimethyl-4-hydroxyphenyl)glutaric acid (III), m. 208-9°
     (EtOAc-petr. ether). Esterification of III by refluxing 12 hrs. with EtOH
     saturated with HCl yielded the ester, m. 158-9° (EtOAc). On refluxing
     2 hrs. with Ac20, III yielded the corresponding anhydride, m.
     230-1° (C6H6-petr. ether). Dry HCl was passed 6 hrs. at
     0-5° through a mixture of 2.4 g. I, 1.2 ml. MeCOCH2CO2Et, and 10 ml.
    HOAc and the mixture kept overnight to yield 1.7 g. Et 3,3-bis(3,5-dimethyl-
     4-hydroxyphenyl)butanoate, m. 147-8° (C6H6-petr. ether). Attempted
    condensation of 2.4 g. I with 1.3 g. Et 2-methylacetoacetate in 10 ml.
    HOAc in the presence of HCl yielded a product, m. 192-3° (EtOAc),
    which could not be characterized. Similar condensation of 2.4 g. I and 2
    ml. ethyl acetonedicarboxylate yielded 400 mg. 2,2-bis(4-hydroxy-3,5-
     dimethylphenyl)propane, m. 161-2°. The reaction of 2,4-xylenol
     (IV) with diethyl oxalacetate Na salt in the presence of concentrated H2SO4 at
     0° yielded a crystalline neutral solid (V), which was identical with
     that obtained by Smith and Bealor (loc. cit.). Concentrated H2SO4 (10 ml.) was
    added dropwise with stirring to a previously cooled (0-5°) mixture of
     2.4 g. IV and 2 ml. ethyl acetonedicarboxylate and the mixture kept
    overnight to yield 1 g. 4-carboxymethyl-6,8-dimethylcoumarin (VI), m.
    206-7°, and 1 g. 4-carbethoxymethyl-6,8-dimethylcoumarin (VII), m.
     100° (EtOAc-petr. ether).
ΙT
    5613-39-8
        (Derived from data in the 7th Collective Formula Index (1962-1966))
RN
     5613-39-8 CAPLUS
CN
    Propionic acid, 3-(3,4-dimethoxyphenyl)-2,2-bis(4-hydroxy-3,5-xylyl)-
     (7CI, 8CI) (CA INDEX NAME)
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L7 ANSWER 10 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1966:93096 CAPLUS DN

64:93096 OREF 64:17468d-f

TIHighly pure hippuran-131I

ΑU Charamza, Otakar; Opavsky, Jiri

CS Fakultni Nemocnice, Olomouc, Czech.

SO Vnitrni Lekarstvi (1965), 11(12), 1211-15

CODEN: VNLEAH; ISSN: 0042-773X

DTJournal

LΑ Czech

AB o-Iodohippuric acid (I) is obtained from o-H2NC6H4CO2H (II) via o-IC6H4CO2H (III) and yields 90% labeled I by ion exchange with Na131I and isolation on a column containing AgCl-sea sand. Thus, a mixture of 30.3 ml. 96% H2SO4, 100 ml. H2O, and 25 g. II is treated at 0° dropwise in 1 hr. with a solution of 12.6 g. NaNO2 in 50 ml. H2O, the brownish solution stirred 30 min. at 0° and 30 g. KI in 50 ml. H2O added with cooling discontinued. The mixture is kept 16 hrs., heated at 60° 30 min. with stirring, shaken with Et20, the product taken up with dilute NaOH, precipitated with HCl, and recrystd. from H2O to give 20

g. III, m. 160-1°. III (10 g.) is refluxed at 80° with fresh SOC12 until evolution of SO2 has ceased (45 min.), the SOC12 distilled in vacuo and with excess C6H6, the residue in C6H6 added dropwise to a mixture of 3 g. H2NCH2CO2H, 2 g. NaOH, and 15 ml. H2O, the mixture stirred 20 min. at <30° with addition of NaOH solution to keep neutral, cooled, and made acid to yield 8.6 g. I, m. 171-4° (H2O). I (0.01-0.1 g.) and 0.1 ml. 0.2% KI is treated in a rubber-stoppered vial with the corresponding amount of Na131I added from a syringe, the mixture kept 2 hrs. in a boiling H2O bath and neutralized at 30-40° with 0.5N NaHCO3. The solution is transferred by means of the syringe onto a column of AgCl-sea sand (1 g.:2 g.) which is then rinsed with 3 ml. physiol. saline. The preparation contains 0.2-0.3 mc./ml. (50  $\mu$ c./mg.) and is ready for use in reno-, splenoporto-, and cerebral circulography after sterilization.

IT 5613-39-8

(Derived from data in the 7th Collective Formula Index (1962-1966))

RN5613-39-8 CAPLUS

CN Propionic acid, 3-(3,4-dimethoxyphenyl)-2,2-bis(4-hydroxy-3,5-xylyl)-(7CI, 8CI) (CA INDEX NAME)

L7 ANSWER 11 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1966:91549 CAPLUS

DN 64:91549

OREF 64:17168e-h

TI Properties and structure of titanium bronzes containing from 0.17 to 5.26 weight % Ti, melted in an induction furnace without the application of an inert atmosphere

AU Gebalski, Stanislaw; Przygodzki, Wieslaw

SO Prace Inst. Mech. Precyzyjnej (1962), 10(4), 23-42

DT Journal

LA Polish

AΒ Five alloys (Cu-Ti) containing 0.17, 1.72, 2.45, 4.25, and 5.26 weight % Ti and impurities 0.5%, rest Cu were melted in an induction furnace in silica-graphite crucibles of capacity 20 kg. with 225,000 frequency and 30 w. power. Copper (Cu 99.9%) was preheated to 500-600° and the flux was introduced whereupon the Cu was melted and heated to 1200°. Afterwards the alloy Cu-Ti with 16.21 weight % Ti was introduced and the temperature was raised to 1250-1300°. The slag was then thickened by the addition of fluorite. The slag was poured off and the alloy was cast at 1260  $\pm$  20° into preheated (to 200°) molds. The ingots were cooled in air, and then placed in stainless steel boxes and packed with charcoal. The protected ingots were then placed into a preheated furnace where they were heated for 6 h. at 900°. The ingots were then cooled in water at 15° then aged for 25 h. at 450°, and cooled in air. Thereafter the tensile strength, elongation, contraction, hardness and microhardness, modulus of elasticity, and coefficient of linear expansion were determined Optimum properties were exhibited by the Cu-Ti alloy containing 2.25-4.25 weight % Ti. A higher content of Ti leads to brittleness without much increase in tensile strength and hardness. The alloys containing 2.45 and 4.25% Ti had after aging the following properties: tensile strength in kg./mm.2, 66 and 75; hardness in kg./mm.2 240 and 200; elongation in 16% and 5, Young's modulus in kg./mm.2, 11,800 and 12,000. The melting of Cu-Ti alloys in air in an induction furnace should be done under a flux which should be thickened; otherwise the metal will contain too high a content of oxide inclusions, and the burn off of Ti will be excessive. The optimum aging conditions were 2 h. at 450° or 8 h. at 430°. 18 refs.

IT 5613-39-8P, Propionic acid, 3-(3,4-dimethoxyphenyl)-2,2-bis(4-hydroxy-3,5-xylyl)-

RL: PREP (Preparation)

(preparation of)

RN 5613-39-8 CAPLUS

CN Propionic acid, 3-(3,4-dimethoxyphenyl)-2,2-bis(4-hydroxy-3,5-xylyl)-(7CI, 8CI) (CA INDEX NAME)

8CI) (CA INDEX NAME)

L7 ANSWER 12 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN ΑN 1935:6099 CAPLUS DN 29:6099 OREF 29:762a-g ΤI Constitution of fustin. II and III. The constitution of hazeic acid (1 and ΑU Oyamada, Taichiro SO Nippon Kagaku Kaishi (1921-47) (1934), 55, 763-74,775-85 CODEN: NIKWAB; ISSN: 0369-4208 DT LΑ Unavailable GI For diagram(s), see printed CA Issue. AB No crystalline product is obtainable from fustin (I) by treating it with dilute acid or alkali, but when methylfustin (II), m. 142-3°, obtained by methylation of I with CH2N2, is treated with dilute alkali, it gives trimethylhazeic acid (III). II with alkali gives 10-20% of 7,3',4'-trimethoxy-3-hydroxyflavone (IV), m. 184-5°, and 40% III, colorless column, m. 138°. III with CH2N2 gives Me tetramethylhazeinate (V), m. 171-2°. V gives tetramethylhazeic acid (VI), m. 188-90°, with dilute alkali, and VI gives V with CH2N2. V and VI are also obtainable by methylation of I with Me2SO4 and alkali (yield 10-40%). III with acid gives anhydrotrimethylhazeyl lactone (VII), C18H16O5, yellow crystals, m. 185°. VII gives anhydrotrimethylhazeic acid (VIII), C18H18O6, on heating several hrs. with alkali. VIII gives Me anhydrotetramethylhazeinate, m. 116°, by diazotation with CH2N2. VI gives a ketone (IX), m. 98.5-9.5°, by the oxidation with KMO4 and the fusion of VI gives anhydrotetramethylhazeic acid, m. 166-8°. The above facts indicate that VI is an  $\alpha HO$  acid having 2 C6H6 nuclei and at least one of the C next to C holding the OH group is not tertiary. The phenolic OH group is in such a position as to form a stable lactone with CO2H; 4 of the O atoms must be in phenolic OH groups since they can easily be methylated by CH2N2 or Me2SO4 and demethylated by HI. The constitution of VI is expressed by 1 of the following formulas: Accordingly III must be VI in which 1 of the 4 OMe groups is replaced by OH. IX gives an oxime (X), C18H21O5N, m. 134-6°, with NH2OH-HCl and alc. KOH. X can be transformed into an amide (XI), m. 120-2°, by PCl5. Saponification of XI gives a homoveratric acid, m. 96-8°, and a dimethoxyaniline, m. 36-8°, which is closest to 2,4-(MeO)2C6H3NH2. The constitution of hazeic acid, therefore, is [2,4-(HO)2C6H3][3,4-(HO)2C6H8CH2] C(OH)CO2H. IT 6600-62-0P, Hazeic acid, trimethyl-RL: PREP (Preparation) (preparation of) RN 6600-62-0 CAPLUS CN Lactic acid, 3-(3,4-dimethoxyphenyl)-2-(2-hydroxy-4-methoxyphenyl)- (7CI,

$$\begin{array}{c|c} \text{OH} & \text{CO}_2\text{H} \\ \hline \text{C} & \text{CH}_2 \\ \hline \text{OH} & \text{OMe} \end{array}$$

=>

AN 1979:203702 CAPLUS

DN 90:203702

OREF 90:32393a,32396a

TI 5-Oxopentanoic acid derivatives

IN Fisnerova, Ludmila; Nemecek, Oldrich; Grimova, Jaroslava

PA Czech.

SO Czech., 6 pp.

CODEN: CZXXA9

DT Patent

LA Czech

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
ΡI	CS 176744	B1	19770630	CS 1975-2824	19750423	
PRAI	CS 1975-2824	Α	19750423			

GΙ

The title compds. I (R1 = H, C3-4 alkyl, C1, NO2, OMe; R2 = H, CHMe2, NMe2, C1, NO2; R3 = Ph, 2-furyl, CMe3, 3-indanyl, C6H3C12-2,4) were prepared by addition of 4-R1C6H4CH2CO2Et to 4-R2C6H4CH:CHCOR3 and saponification of the product. Thus, a solution of 2.46 g PhCH2CO2Et and 3.7 g 4-Me2CHC6H4CH:CHCOPh in Et2O containing EtONa was kept 5 days to give 4.4 g PhCOCH2CH(C6H4CHMe2-4)CHPhCO2Et which was refluxed with AcOH-HBr to yield 3.5 g I (R1 = H, R2 = CHMe2, R3 = Ph). Similarly prepared were PhCOCH2CHR4CHR5CO2H (R4 = 2-pyrrolyl, 3-pyridyl; R5 = Ph, C6H4NO2-4, C6H4CH2CHMe2-4).

IT 59771-47-0P 59771-91-4P 70334-43-9P 70334-44-0P 70334-45-1P 70334-46-2P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RN 59771-47-0 CAPLUS

CN Benzenepentanoic acid,  $\beta$ -[4-(1-methylethyl)phenyl]- $\alpha$ -[4-(1-methylpropyl)phenyl]- $\delta$ -oxo-, ethyl ester (9CI) (CA INDEX NAME)

RN 59771-91-4 CAPLUS

CN Benzenepentanoic acid,  $\beta$ -[4-(1-methylethyl)phenyl]- $\alpha$ -[4-(1-methylpropyl)phenyl]- $\delta$ -oxo- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ &$$

RN 70334-43-9 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -(3,3-dimethyl-2-oxobutyl)-4-(1-methylethyl)- $\alpha$ -[4-(2-methylpropyl)phenyl]-, ethyl ester (CA INDEX NAME)

RN 70334-44-0 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -(3,3-dimethyl-2-oxobutyl)-4-(1-methylethyl)- $\alpha$ -[4-(2-methylpropyl)phenyl]- (CA INDEX NAME)

$$CH_2-C-Bu-t$$
 $CO_2H$ 
 $CH-CH-CH$ 
 $Bu-i$ 

RN 70334-45-1 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -(3,3-dimethyl-2-oxobutyl)-4-(1-methylethyl)- $\alpha$ -[4-(1-methylethyl)phenyl]-, ethyl ester (CA INDEX NAME)

RN 70334-46-2 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -(3,3-dimethyl-2-oxobutyl)-4-(1-methylethyl)- $\alpha$ -[4-(1-methylethyl)phenyl]- (CA INDEX NAME)

=>

ANSWER 128 OF 267 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1985:45575 CAPLUS

DN 102:45575

OREF 102:7157a,7160a

TI Synthetic studies in polycyclic systems: part IX - synthesis of methoxy derivatives of 11H-benzo[a]fluorenes and 11H-naphtho[2,1-a]fluorenes

AU Rao, Alaka; Lala, Sunandan; Rao, R. R.

CS Dep. Chem., Visva-Bharati Univ., Santiniketan, 731 235, India

SO Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1984), 23B(7), 603-10

CODEN: IJSBDB; ISSN: 0376-4699

DT Journal

LA English

OS CASREACT 102:45575

GΙ

$$R^{2}$$
 $R^{3}$ 
 $R^{2}$ 
 $R^{2}$ 
 $R^{3}$ 
 $R^{2}$ 
 $R^{3}$ 
 $R^{2}$ 
 $R^{3}$ 
 $R^{4}$ 
 $R^{5}$ 
 $R^{6}$ 
 $R^{1}$ 

AB Michael reaction of RCH:CHCO2Et [R = C6H4OMe-2, -3, -3,C6H3COMe)2-3,4] with R1CH2CO2Et (R1 = Ph, 2-naphthyl) gave 75-86% EtO2CCHR1CHRCH2CO2Et, which was hydrolyzed to give HO2CCHR1CNRCH2CO2H. The diacids were cyclized with SnCl4 to give 54-64% tetralone derivs. I (R2 = R3 = H, CH:CHCH:CH; X = O) which were reduced with Zn or H2NNH2 to give 58-67, 59-66% I (X = H2) resp. The last were methylated, dehydrogenated, and saponified to give naphthalene- and phenanthrenecarboxylic acids II (same R's), which were cyclized using H2SO4, AlCl3, or SnCl4 to give 18-38, 29-42, 52-74% fluorenone derivs. III (R4 = R6 = OMe, R3 = H; R4 = OMe, R5 = R6 = H; R4 = R6 = H, R5 = OMe; R4 = R5 = H, R6 = OMe, X6 = O), resp. The ketones were reduced with H2NNH2 to give 54-67% title compds. III (same R's, X1 = H2).

IT 94146-62-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and saponification of)

RN 94146-62-0 CAPLUS

IT 94146-18-6P 94146-19-7P 94146-20-0P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RN 94146-18-6 CAPLUS

CN Pentanedioic acid, 2-(2-carboxyphenyl)-3-(3-methoxyphenyl)- (CA INDEX NAME)

RN 94146-19-7 CAPLUS

CN Pentanedioic acid, 2-(2-carboxyphenyl)-3-(4-methoxyphenyl)- (CA INDEX NAME)

RN 94146-20-0 CAPLUS

CN Pentanedioic acid, 2-(2-carboxyphenyl)-3-(3,4-dimethoxyphenyl)- (CA INDEX NAME)

IT 94146-63-1P 94146-64-2P 94146-65-3P

94146-66-4F

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation, hydrolysis, and Dieckmann cyclization of)

RN 94146-63-1 CAPLUS

CN Pentanedioic acid, 2-[2-(ethoxycarbonyl)phenyl]-3-(3-methoxyphenyl)-, diethyl ester (9CI) (CA INDEX NAME)

## > d his

(FILE 'HOME' ENTERED AT 08:08:15 ON 27 DEC 2007)

FILE 'REGISTRY' ENTERED AT 08:08:27 ON 27 DEC 2007

L1STRUCTURE UPLOADED

L2 1 S L1

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L41 S L1 CSS FUL

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L4 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2007 ACS on STN

RN 353228-00-9 REGISTRY

ED Entered STN: 28 Aug 2001

CN Benzenepropanoic acid, α-(4-hydroxyphenyl)-3,4-dimethoxy- (CA INDEX NAME)

C17 H18 O5 MF

SR CA

LCSTN Files: CA, CAPLUS, TOXCENTER, USPATFULL

$$\begin{array}{c|c} \text{OMe} & \text{OMe} \\ \hline \text{CO}_2\text{H} & \text{OMe} \\ \hline \text{CH-CH}_2 & \text{OMe} \end{array}$$

# \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

# REFERENCE 1

AN

ΤI Preparation of diphenylethylene compounds as antidiabetic agents

IN Nag, Bishwagit; Dey, Debendranath; Medicherla, Satyanarayana; Neogi, Partha

PA USA

U.S. Pat. Appl. Publ., 38 pp., Cont.-in-part of U.S. Ser. No. 642,618. SO CODEN: USXXCO

DT Patent

LΑ English

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	PATENT NO.	KIND	DATE	PPLICATION NO.	DATE				
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ΡI	US 2002002200	A1	20020103	U	S 2001-777551	20010205			
	US 6624197	B1	20030923	U	S 2000-642618	20000817			
	US 2004097593	A1	20040520	U	S 2003-430677	20030507			
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TI
     Novel diphenylethylene compounds
     Nag, Bishwajit; Dey, Debendranath; Medicherla, Satyanarayana
IN
     Calyx Therapeutics, Inc., USA
PA
     PCT Int. Appl., 55 pp.
SO
     CODEN: PIXXD2
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RE.CNT 7
             THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD
             ALL CITATIONS AVAILABLE IN THE RE FORMAT
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